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AUTHOR(S):

Mitsui, Taketomo

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Runge-Kutta Type Integration Formulas  
Including the Evaluation of the Second Derivative

Part I

Taketomo MITSUI  
Research Institute for Mathematical Sciences  
Kyoto University, Kyoto.

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## Introduction

We are concerning with theoretical study of numerical integration procedure for the initial-value problem of ordinary differential equation:

$$(E) \quad \frac{dy}{dx} = f(x, y),$$

$$(IV) \quad y(x_I) = y_I.$$

Many numerical analysts have been investigating the discrete variable methods for the problem. Consequently everyone can enjoy to solve ordinary differential equation in almost all computing centers. It seems as if we got the numerical integrator through the use of the computer. But the study is yet continued for "better" numerical procedure

Among the one-step methods, Runge-Kutta methods (RK methods, in short) are popular because of the high accuracy and the feasibility of changing step-size. In general the methods are expressed as follows. The solution of (E) at  $x_0+h$  is approximated by

$$y_1 = y_0 + h \sum_{i=1}^p \mu_i k_i,$$

where

$$\begin{aligned} k_1 &= f(x_0, y_0), \\ (*) \quad k_i &= f(x_0 + \alpha_i h, y_0 + h \sum_{j=1}^{i-1} \beta_{ij} k_j), \quad i = 2, \dots, p, \end{aligned}$$

$h$  is the step-size and  $y_0$  is the approximated value at

$x_0$ . This type of the method is called (explicit) p-stage Runge-Kutta algorithm. According to the choice of the stage number  $p$  and the parameters  $\alpha_i, \beta_{ij}, \nu_i$  we have many variations, among which the classical Runge-Kutta method or the Runge-Kutta-Fehlberg method is famous. A distinguished contribution for the study of the Runge-Kutta methods has been made by J. C. Butcher ([1] ~ [4]). He determined the attainable order of the RK methods up to 10-stage formula. On the other hand he introduced the semi-explicit (the summation is up to  $i$  instead of  $i-1$  in (\*)) or implicit (the summation is up to  $p$  in (\*)) formula.

RK methods (and perhaps many other quadrature formulas for the initial-value problem) are constructed on the principle that the required function evaluation is only for  $f(x,y)$ , i.e. the first derivative of the solution. It is quite natural because we are acquainted with the functional form of the first derivative in the ordinary differential equation. Recently, however, some propositions have been made to employ the function evaluation of the second derivative of the solution. Functional form of it is given by

$$g(x,y) = f_x(x,y) + f_y(x,y)f(x,y).$$

M. Urabe [15] made a first attempt to employ  $g(x,y)$  by presenting an implicit one-step method with step-size control strategy. Let  $y_0$  and  $y_{-1}$  be approximations of  $y(x)$  at  $x_0$  and  $x_0-h$ , respectively. His algorithm employs the predictor given by

$$\hat{y}_1 = -31y_{-1} + 32y_0 - h(14f_{-1} + 16f_0) + h^2(-2g_{-1} + 4g_0)$$

and the corrector given by

$$y_0 = y_{-1} + \frac{h}{240}(101f_{-1} + 128f_0 + 11f_1) \\ + \frac{h^2}{240}(13g_{-1} - 40g_0 - 3\hat{g}_1),$$

where  $f_i = f(x_0+ih, y_i)$ ,  $g_i = f(x_0+ih, y_i)$ ,  $\hat{f}_1 = f(x_0+h, y_1)$  and  $\hat{g}_1 = g(x_0+h, y_1)$ . Succeeding his result, J. R. Cash [5] has considered this type of formula more generally and made some stability analysis. On the other hand H. Shintani [12], [13] has proposed some formulas analogous to RK formula employing one evaluation for  $f(x, y)$  and some for  $g(x, y)$ . He has given the values of the parameters appearing in the formulas up to the order 7. His results, closely related to the present work, will be mentioned afterward.

In this context another type of integration formula, for the origination of which H. H. Rosenbrook [11] is given credit, is now being developed. It employs the partial derivative  $f_y(x, y)$  and is reported to have good stability for stiff systems of ordinary differential equations ([7], [9]).

Here we shall examine an explicit  $(p, q)$ -stage Runge-Kutta type formula including the second derivative. It requires  $p$  times evaluations for the first derivative and  $q$  times for the second derivative in a similar manner for RK methods. We are interested in the following problems

- (1) What is the attainable order of the  $(p, q)$ -stage formula from the viewpoint of its local accuracy?
- (2) How are the parameters in the formula determined?
- (3) What formula is good for practical use?

These problems will be solved in the following sections and the forthcoming paper by the author. The present paper is especially devoted to investigate the  $(1,q)$ -stage formulas

First, we shall define explicit  $(p,q)$ -stage formula. Next, some algebraic computations are carried out to investigate  $(p,q)$ -stage formulas. Here SAM software is used as a powerful tool. Then, the attainable order of  $(1,q)$ -stage formula is determined up to  $q=4$

Remark. In the case of very complicated functional form of  $f(x,y)$  in higher dimension, the calculation of the second derivative  $g(x,y)$  requires a laborious work. It is the main reason why the methods employing  $g(x,y)$  have not been considered. But the recent development of the symbolic and algebraic manipulation (SAM) software brings the change of the situation. SAM software, for example, REDUCE-2 or MACSYMA, is now a helpful tool for mathematical sciences. In fact, some SAM program may print expressions in a FORTRAN notation so that one can carry out the calculation of the second derivative from  $f(x,y)$  in an automatic way. Once after algebraic computation we may call  $g(x,y)$  as a FUNCTION subprogram.

Moreover, SAM software is very useful for the theoretical study of the RK and its analogous methods. For example, H. Toda [14] has considered 5-stage RK limiting formula of order 5. He has utilized MACSYMA essentially. We shall also attempt to apply SAM for our study.

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### §1.1 Explicit (p,q)-Stage Formula

We shall discuss numerical integration procedure for the initial-value problem of ordinary differential equation:

$$(1.1.1) \quad \frac{dy}{dx} = f(x,y),$$

$$(1.1.2) \quad y(x_I) = y_I.$$

Here  $f$  is sufficiently smooth with respect to  $x$  and  $y$ . Let us define an explicit (p,q)-stage Runge-Kutta type formula including the second derivative of the solution. Let  $g$  stand for the second derivative of  $y(x)$ ,

$$(1.1.3) \quad g(x,y) = f_x(x,y) + f_y(x,y)f(x,y)$$

Explicit (p,q)-stage formula is given as follows

$$(1.1.4) \quad y_{n+1} = y_n + h \sum_{i=1}^p \mu_i k_i + h^2 \sum_{i=1}^q \nu_i K_i, \quad n=0,1,2, \dots,$$

where

$$(1.1.5) \quad \begin{cases} k_1 = f(x_n + \alpha_1 h, y_n), \\ k_i = f(x_n + \alpha_i h, y_n + h \sum_{j=1}^{i-1} \beta_{ij} k_j + h^2 \sum_{j=1}^{i-1} \gamma_{ij} K_j), \quad i=2, \dots, p, \end{cases}$$

$$(1.1.6) \quad \begin{cases} K_1 = g(x_n + \rho_1 h, y_n + h \sigma_{11} k_1), \\ K_i = g(x_n + \rho_i h, y_n + h \sum_{j=1}^i \sigma_{ij} k_j + h^2 \sum_{j=1}^{i-1} \tau_{ij} K_j), \quad i=2, \dots, q \end{cases}$$

Remark 1. The parameters  $\mu_i, \nu_i, \alpha_i, \beta_{ij}, \gamma_{ij}, \rho_i, \sigma_{ij}$  and  $\tau_{ij}$  are, of course, real numbers

Remark 2. In the case of simultaneous equations in (1),  $y$  and  $f$  are considered vectors of the same dimension. Then  $f_y(x,y)$ , the Jacobian matrix of  $f$ , is given in the matrix form. For example, assume that

$$f(x,y) = \begin{bmatrix} f_1(y_1, y_2) \\ f_2(y_1, y_2) \end{bmatrix} = \begin{bmatrix} (a_1 - b_1 y_2) y_1 \\ (a_2 - b_2 y_1) y_2 \end{bmatrix}$$

where  $a_i$  and  $b_i$  are constants, then

$$f_y(x,y) = \begin{bmatrix} a_1 - b_1 y_2 & -b_1 y_1 \\ -b_2 y_2 & a_2 - b_2 y_1 \end{bmatrix}$$

and

$$g(x,y) = \begin{bmatrix} a_1^2 y_1 + (b_2 y_1 + b_1 y_2 - 2a_1 - a_2) b_1 y_1 y_2 \\ a_2^2 y_2 + (b_2 y_1 + b_1 y_2 - a_1 - 2a_2) b_2 y_1 y_2 \end{bmatrix}$$

Similar to the RK formulas, the determining equations and the parameters are possible to be slightly different between the single differential equation and the systems of equations. For convenience sake we shall investigate the single case. The attainable order of the formula is not depend on whether (1) is single or system.

## §1.2 The Taylor Series Expansion of the Solution

To investigate Runge-Kutta type methods of higher order, we are required to represent the solution  $y(x_0+h)$  for (E) and (IV) in §1.1 into the power series of the stepsize  $h$ . For our quadrature formula it is preferable to represent the solution into the power series utilizing the second derivative  $g$ .

Twice integration after differentiation for the equation

$$\frac{dy}{dx} = f(x, y), \quad x \geq x_0$$

implies the formula

$$(1.2.1) \quad \int_{x_0}^{x_0+h} \left\{ \int_{x_0}^t \frac{d^2 y(x)}{dx^2} dx \right\} dt = \int_{x_0}^{x_0+h} \left\{ \int_{x_0}^t g(x, y(x)) dx \right\} dt.$$

The left-hand side of the above formula is equal to

$$\begin{aligned} & y(x_0+h) - y(x_0) - hf(x_0, y(x_0)) \\ &= y(x_0+h) - y_0 - hf_0. \end{aligned}$$

Hereafter the subscript 0 stands for the evaluation at  $x = x_0$  and  $y = y_0$

The right-hand side of (1) becomes

$$\int_0^h \left\{ \int_{x_0}^{x_0+\xi} g(x, y(x)) dx \right\} d\xi = \int_0^h \left\{ \int_0^\xi g(x_0+\zeta, y(x_0+\zeta)) d\zeta \right\} d\xi$$

Then, assume that for  $0 \leq \zeta \leq h$   $y(x_0 + \zeta)$  can be expanded in the power series of  $\zeta$  by

$$(1.2.2) \quad y(x_0 + \zeta) = y_0 + \zeta f_0 + \sum_{r=2}^m \frac{\kappa_{r-2}}{r!} \zeta^r + O(\zeta^{m+1}),$$

where  $\kappa_j$  ( $j=1,2, \dots, m$ ) is the coefficient to be determined later. Substitution (2) into the integrand implies

$$\begin{aligned} g(x_0 + \zeta, y(x_0 + \zeta)) &= g(x_0 + \zeta, y_0 + \zeta f_0 + \sum_{r=2}^m \frac{\kappa_{r-2}}{r!} \zeta^r + O(\zeta^{m+1})) \\ &= \sum_{\ell=0}^m \frac{1}{\ell!} [(\zeta \frac{\partial}{\partial x} + (\zeta f_0 + \sum_{r=2}^m \frac{\kappa_{r-2}}{r!} \zeta^r) \frac{\partial}{\partial y})^\ell g]_0 + O(\zeta^{m+1}) \\ &= \sum_{\ell=0}^m \frac{\zeta^\ell}{\ell!} [D_0 + (\sum_{r=2}^m \frac{\kappa_{r-2}}{r!} \zeta^{r-1}) \frac{\partial}{\partial y}]^\ell g|_0 + O(\zeta^{m+1}) \\ &= \sum_{\ell=0}^m \frac{\zeta^\ell}{\ell!} \{ \sum_{k=0}^{\ell} \binom{\ell}{k} (\sum_{r=1}^{m-1} \frac{\kappa_{r-1}}{(r+1)!} \zeta^r)^k \\ &\quad \times [D_0^{\ell-k} (\frac{\partial}{\partial y})^k g]_0 \} + O(\zeta^{m+1}) \end{aligned}$$

Here  $D_0$  is a differential operator defined by

$$D_0 = \frac{\partial}{\partial x} + f_0 \frac{\partial}{\partial y}.$$

Therefore we have the following equation:

$$\begin{aligned} (1.2.3) \quad y_0 + hf_0 + \sum_{r=2}^{m+2} \frac{\kappa_{r-2}}{r!} \zeta^r &= y_0 + hf_0 + \\ &+ \int_0^h \left( \int_0^\xi \sum_{\ell=0}^m \frac{\zeta^\ell}{\ell!} \{ \sum_{k=0}^{\ell} \binom{\ell}{k} (\sum_{r=1}^{m-1} \frac{\kappa_{r-1}}{(r+1)!} \zeta^r)^k [D_0^{\ell-k} (\frac{\partial}{\partial y})^k g]_0 \} d\zeta \right) d\xi, \end{aligned}$$

which determines  $\kappa_j$  recurrently.

Twice differentiation for (3) with respect to  $h$  implies

$$(1.2.4) \quad \sum_{\ell=0}^m \frac{\kappa_{\ell}}{\ell!} h^{\ell} = \sum_{\ell=0}^m \frac{h^{\ell}}{\ell!} \left\{ \sum_{k=0}^{\ell} \binom{\ell}{k} \left( \sum_{r=1}^{m-1} \frac{\kappa_{r-1}}{(r+1)!} h^r \right)^k \times \right. \\ \left. \times [D_0^{\ell-k} (\frac{\partial}{\partial y})^k g]_0 \right\}$$

Then, we have the following important result.

Theorem 1. The coefficient  $\kappa_{\ell}$  ( $\ell=0,1, \dots, m$ ) is determined by the following way:

$$(1.2.5) \quad \begin{cases} \kappa_0 = g_0. \\ \kappa_{\ell} = [D_0^{\ell} g]_0 + \sum_{s=1}^{\ell-1} \left\{ \sum_{t=1}^{m(\ell,s)} \frac{\ell!}{s!(\ell-s-t)!} \times \right. \\ \left. \times B_{s,t} \left( \frac{\kappa_0}{2}, \frac{\kappa_1}{3}, \dots, \frac{\kappa_{s-1}}{s+1} \right) [D_0^{\ell-s-t} (\frac{\partial}{\partial y})^t g]_0 \right\}, \end{cases}$$

for  $\ell=1,2, \dots, m$ .

Here  $B_{s,t}(x_1, x_2, \dots, x_s)$  is the multivariable polynomial of E. T. Bell of the order  $(s,t)$  and

$$m(\ell,s) \equiv \min(s, \ell-s)$$

Note.  $\kappa_j$  appeared in the summation of the right-hand side of (5) is for  $j$  less than or equal to  $\ell-2$  so that we can determine  $\kappa_{\ell}$  recurrently by the formula.

Proof  $\kappa_0 = g_0$  is clear. Let us introduce two

functions  $G(h)$  and  $A(h; \ell)$  as follows:

$$(1.2.6) \quad G(h) = \sum_{r=1}^{m-1} \frac{\kappa_{r-1}}{(r+1)!} h^r,$$

$$(1.2.7) \quad A(h; \ell) = \sum_{k=0}^{\ell} \binom{\ell}{k} [G(h)]^k [D_0^{\ell-k} (\frac{\partial}{\partial y})^k g]_0, \quad \ell=0,1,\dots,m.$$

Note that  $G(h)$  is of the order  $h$  and  $G(0) = 0$  holds

Then, the right-hand side of (4) is equal to  $\sum_{s=0}^m \frac{A(h;s)}{s!} h^s$

Hence, we have the equation

$$(1.2.8) \quad \sum_{\ell=0}^m \frac{\kappa_{\ell}}{\ell!} h^{\ell} = \sum_{s=0}^m \frac{A(h;s)}{s!} h^s$$

For an integer  $\ell$  such that  $1 \leq \ell \leq m$ ,  $\ell$ -times differentiation to (8) with respect to  $h$  implies

$$(1.2.9) \quad \kappa_{\ell} = \sum_{s=0}^{\ell-1} \binom{\ell}{s} A^{(s)}(0; \ell-s)$$

By (7), the equation

$$A(0; \ell) = [D_0^{\ell} g]_0$$

is clear. For  $s \geq 1$ , we have from (7)

$$\begin{aligned} A^{(s)}(h; \ell-s) &= \binom{\ell-s}{1} G^{(s)}(h) [D_0^{\ell-s-1} g_y]_0 + \\ &+ \binom{\ell-s}{2} \frac{d^s}{dh^s} \{G(h)\}^2 [D_0^{\ell-s-2} g_{yy}]_0 + \dots + \\ &+ \binom{\ell-s}{k} \frac{d^s}{dh^s} \{G(h)\}^k [D_0^{\ell-s-k} (\frac{\partial}{\partial y})^k g]_0 + \dots + \\ &+ \frac{d^s}{dh^s} \{G(h)\}^{\ell-s} [(\frac{\partial}{\partial y})^{\ell-s} g]_0 \end{aligned}$$

For higher derivatives of composite functions, the formula employing the Bell polynomial is known (J. Riordan [10]). Hence, applying the formula, we have for  $k=1,2,\dots,l-s$

$$\frac{d^s}{dh^s}\{G(h)\}^k = \sum_{t=1}^{\min(s,k)} \frac{k!}{(k-t)!} B_{s,t}(G'(h), G''(h), \dots, G^{(s)}(h)) \times \\ \times \{G(h)\}^{k-t},$$

which implies

$$\left\{ \frac{d^s}{dh^s}\{G(h)\}^k \right\}_{h=0} = \begin{cases} k! B_{s,k}(G'(0), G''(0), \dots, G^{(s)}(0)) & \text{for } s \leq k, \\ 0 & \text{for } s > k. \end{cases}$$

From (6), the equation

$$G^{(s)}(h) = \sum_{r=s}^{m-1} \frac{r!}{(r-s)!} \frac{\kappa_{r-1}}{(r+1)!} h^{r-s} = \sum_{r=s}^{m-1} \frac{\kappa_{r-1}}{(r+1)!(r-s)!} h^{r-s}$$

holds. Hence we have

$$G^{(s)}(0) = \frac{\kappa_{s-1}}{s+1}, \quad s=1,2,\dots,m-1.$$

Then  $A^{(s)}(0; l-s)$  is given by

$$A^{(s)}(0, l-s) = \sum_{k=1}^{m(l,s)} \binom{l-s}{k} k! B_{s,t}(G'(0), \dots, G^{(s)}(0)) [D_0^{l-s-k} (\frac{\partial}{\partial y})^k g]_0 \\ = \sum_{t=1}^{m(l,s)} \frac{(l-s)!}{(l-s-t)!} B_{s,t}(\frac{\kappa_0}{2}, \frac{\kappa_1}{3}, \dots, \frac{\kappa_{s-1}}{s+1}) [D_0^{l-s-t} (\frac{\partial}{\partial y})^t g]_0,$$

which implies from (9)

$$\begin{aligned}
\kappa_\ell &= [D_0^\ell g]_0 + \sum_{s=1}^{\ell-1} \binom{\ell}{s} \left\{ \sum_{t=1}^{m(\ell,s)} \frac{(\ell-s)!}{(\ell-s-t)!} B_{s,t} \left( \frac{\kappa_0}{2}, \frac{\kappa_1}{3}, \dots, \frac{\kappa_{s-1}}{s+1} \right) \times \right. \\
&\quad \left. \times [D_0^{\ell-s-t} \left( \frac{\partial}{\partial y} \right)^t g]_0 \right\} \\
&= [D_0^\ell g]_0 + \sum_{s=1}^{\ell-1} \left\{ \sum_{t=1}^{m(\ell,s)} \frac{\ell!}{s!(\ell-s-t)!} B_{s,t} \left( \frac{\kappa_0}{2}, \frac{\kappa_1}{3}, \dots, \frac{\kappa_{s-1}}{s+1} \right) \times \right. \\
&\quad \left. \times [D_0^{\ell-s-t} \left( \frac{\partial}{\partial y} \right)^t g]_0 \right\}
\end{aligned}$$

This is the desired result.  $\square$

The multivariable polynomial  $B_{s,t}(x_1, x_2, \dots, x_s)$  has a recurrence formula to calculate it conveniently by the application of any SAM software. That is,

$$\begin{aligned}
&\sum_{t=1}^s x_1 B_{s,t}(x_1, \dots, x_s) a^{t+1} + \sum_{t=1}^s \left( \sum_{k=1}^s x_{k+1} \frac{\partial B_{s,t}}{\partial x_k} \right) a^t \\
&= \sum_{t=1}^{s+1} B_{s+1,t}(x_1, \dots, x_{s+1}) a^t
\end{aligned}$$

Here, the both sides of the formula is considered as a polynomial of  $a$ . The recurrence formula for  $B_{s,t}$  will be employed during the calculations of  $\kappa_\ell$  by REDUCE-2

Theorem 1 tells us a concrete method to determine the Taylor series expansion (2) employing the second derivative. For example,

$$\kappa_1 = [D_0 g]_0,$$



$$\kappa_2 = [D_0^2 g]_0 + 2! B_{1,1} \left(\frac{\kappa_0}{2}\right) g_{y,0} = [D_0^2 g]_0 + \kappa_0 g_{y,0}$$

$$= [D_0^2 g]_0 + g_0 g_{y,0},$$

$$\kappa_3 = [D_0^3 g]_0 + 3! B_{1,1} \left(\frac{\kappa_0}{2}\right) [D_0 g_y]_0 + \frac{3!}{2!} B_{2,1} \left(\frac{\kappa_0}{2}, \frac{\kappa_1}{3}\right) g_{y,0}$$

$$= [D_0^3 g]_0 + 3\kappa_0 [D_0 g_y]_0 + \kappa_1 g_{y,0}$$

$$= [D_0^3 g]_0 + 3g_0 [D_0 g_y]_0 + [D_0 g]_0 g_{y,0}.$$

We may also carry out the process by the SAM software up to the desired order. The result by REDUCE-2 is shown in Table 1.

Note that because of Remark 2 in the preceding section we do not care the order of the higher partial derivatives.

Another important result from Theorem 1 is that any  $\kappa_j$  is a summation of an integer multiple of some product of  $[D_0^p (\frac{\partial}{\partial y})^q g]_0$ . Hence, we shall call any product of  $[D_0^p (\frac{\partial}{\partial y})^q g]_0$  an elementary differential of  $g$ . J. C. Butcher [1] has used the terminology of elementary differential in a different sense. However, our study of the expression of the coefficient of Taylor series in the elementary differentials is on the similar point of view.

In fact, the way of the proof of Theorem 1 is applicable to the Taylor series expansion of  $y(x_0+h)$  employing the first derivative.

Theorem 2 Assume that

$$(1.2.10) \quad y(x_0+h) = y_0 + \sum_{r=1}^m \frac{\lambda_{r-1}}{r!} h^r + O(h^{m+1}).$$

Then, the coefficient  $\lambda_\ell$  ( $\ell=0,1,\dots,m-1$ ) is determined by

$$(1.2.11) \quad \begin{cases} \lambda_0 = f_0 \\ \lambda_\ell = [D_0^\ell f]_0 + \sum_{s=1}^{\ell-1} \left\{ \sum_{t=1}^{m(\ell,s)} \frac{\ell!}{(\ell-s-t)!s!} \times \right. \\ \quad \times B_{s,t} \left( \frac{\lambda_1}{2}, \frac{\lambda_2}{3}, \dots, \frac{\lambda_s}{s+1} \right) [D_0^{\ell-s-t} \left( \frac{\partial}{\partial y} \right)^t f]_0 \Big\}, \\ \ell = 1, 2, \dots, m. \end{cases}$$

We shall call (10) the first type power series expansion in contrast with (2) which will be mentioned as the second type expansion.

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Table 1

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### §1.3 Implicit (1,q)-Stage Formula.

For the study of the general (1,q)-stage formula, it is convenient to analyse the corresponding implicit (1,q)-stage formula, because we gain an insight into its algebraic relations by them.

Consider an implicit (1,q)-stage formula as follows:

$$(1.3.1) \quad y_{n+1} = y_n + \mu_1 h k_1 + \sum_{i=1}^q \nu_i h^2 K_i, \quad n = 0, 1, 2, \dots,$$

$$(1.3.2) \quad \begin{cases} k_1 = f(x_n + \alpha_1 h, y_0), \\ K_i = g(x_n + \rho_i h, y_n + \sigma_{i1} h k_1 + \sum_{j=1}^q \tau_{ij} h^2 K_j), \quad i = 1, \dots, q. \end{cases}$$

We need to analyse one-step integration by (1) and (2), so we may substitute  $n=0$ , i.e.

$$(1.3.3) \quad \begin{cases} y_1 = y_0 + \mu_1 h k_1 + \sum_{i=1}^q \nu_i h^2 K_i, \\ k_1 = f(x_0 + \alpha_1 h, y_0), \\ K_i = g(x_0 + \rho_i h, y_0 + \sigma_{i1} h k_1 + \sum_{j=1}^q \tau_{ij} h^2 K_j), \quad i = 1, \dots, q \end{cases}$$

For  $k_1$ , we have the following expansion:

$$k_1 = f_0 + \alpha_1 h f_{x,0} + \frac{1}{2} \alpha_1^2 h^2 f_{xx,0} + O(h^3)$$

On the other hand,  $K_1$  has the expansion

$$K_1 = g_0 + O(h)$$

Hence, the equation

$$(1.3.4) \quad y_1 = y_0 + \mu_1 h f_0 + h^2 (\mu_1 \alpha_1 f_{x,0} + \sum_{i=1}^q v_i g_0) + O(h^3)$$

holds. The solution  $y(x_0+h)$  has the power series of  $h$  as follows:

$$(1.3.5) \quad y(x_0+h) = y_0 + h f_0 + \frac{1}{2} h^2 g_0 + O(h^3)$$

Comparison of the terms having the same power of  $h$  in (4) and (5) yields the following equations.

$$\mu_1 = 1,$$

$$\mu_1 \alpha_1 f_{x,0} + \sum_{i=1}^q v_i g_0 = \frac{1}{2} g_0.$$

Thus,  $\mu_1=1$ ,  $\alpha_1=0$  and  $\sum_{i=1}^q v_i = \frac{1}{2}$  must hold in the implicit (1,q)-stage formula.

Next, since  $K_1$  has the expansion

$$K_1 = g_0 + [(\rho_{1\frac{\partial}{\partial x}} + \sigma_{11} f_0 \frac{\partial}{\partial y})g]_0 h + O(h^2),$$

the comparison of the third order term of  $y_1$  and  $y(x_0+h)$  implies the equation.

$$\frac{1}{2} [D_0 g]_0 = \frac{1}{2} (g_{x,0} + f_0 \cdot g_{y,0}) = \sum_{i=1}^q v_i [(\rho_i g_{x,0} + \sigma_{i1} f_0 \cdot g_{y,0})]$$

From the viewpoint of homogeneity of differential operation,

$\rho_i = \sigma_{i1}$  must hold for  $i=1, 2, \dots, q$

Hence, let us rewrite (3) by

$$(1.3.6) \quad \begin{cases} y_1 = y_0 + hf_0 + \sum_{i=1}^q v_i h^2 k_i, \\ K_i = g(x_0 + \rho_i h, y_0 + \rho_i hf_0 + \sum_j \tau_{ij} h^2 K_j), \quad i = 1, \dots, q. \end{cases}$$

We shall assume the Taylor series expansion for  $K_i$  by

$$(1.3.7) \quad K_i = \sum_{\ell=0}^m \frac{\kappa_{i\ell}}{\ell!} h^\ell + O(h^{m+1}),$$

where  $\kappa_{i\ell}$  will be determined by the similar manner for Theorem 1.

Theorem 3. For each  $i$ ,  $\kappa_{i\ell}$  in (1.3.7) is determined by the following:

$$(1.3.8) \quad \begin{cases} \kappa_{i0} = g_0, \\ \kappa_{i\ell} = \rho_i^\ell [D_0^\ell g]_0 + \sum_{s=1}^{\ell-1} \left\{ \sum_{t=1}^{m(\ell,s)} \frac{\ell!}{s!(\ell-s-t)!} \rho_i^{\ell-s-t} \right. \\ \quad \times B_{s,t} \left( \sum_{j=1}^q \tau_{ij} \kappa_{j0}, \dots, s \sum_{j=1}^q \tau_{ij} \kappa_{j,s-1} \right) \\ \quad \left. \times [D_0^{\ell-s-t} \left( \frac{\partial}{\partial y} \right)^t g]_0 \right\}, \quad \ell = 1, 2, \dots, m. \end{cases}$$

Note. By the above formula,  $\kappa_{i\ell}$  can be determined in the ascending order of the second subscript, i.e.,  $\kappa_{i2}$  ( $i=1, \dots, q$ ) after  $\kappa_{11}$ ,  $\kappa_{i3}$  ( $i=1, \dots, q$ ) after  $\kappa_{i2}$ , and so on.

Proof. Two-variable Taylor series expansion for  $K_1$  gives

$$\begin{aligned} K_1 &= \sum_{\ell=0}^m \frac{1}{\ell!} \left[ \left\{ \rho_1 h \frac{\partial}{\partial x} + (\rho_1 h f_0 + \sum_{j=1}^q \tau_{1j} h^2 K_j) \frac{\partial}{\partial y} \right\}^\ell g \right]_0 + O(h^{m+1}) \\ &= \sum_{\ell=0}^m \frac{h^\ell}{\ell!} \left[ \left\{ \rho_1 D_0 + \left( \sum_{j=1}^q \tau_{1j} h K_j \right) \frac{\partial}{\partial y} \right\}^\ell g \right]_0 + O(h^{m+1}) \\ &= \sum_{\ell=0}^m \frac{h^\ell}{\ell!} \left[ \left\{ \rho_1 D_0 + \left( \sum_{r=0}^{m-1} \left( \sum_{j=1}^q \frac{\tau_{1j} \kappa_{jr}}{r!} \right) h^{r+1} \right) \frac{\partial}{\partial y} \right\}^\ell g \right]_0 + O(h^{m+1}) \\ &= \sum_{\ell=0}^m \frac{h^\ell}{\ell!} \left\{ \sum_{k=0}^{\ell} \binom{\ell}{k} \rho_1^{\ell-k} \left( \sum_{r=0}^{m-1} \left( \sum_{j=1}^q \frac{\tau_{1j} \kappa_{jr}}{r!} \right) h^{r+1} \right)^k [D_0^{\ell-k} \left( \frac{\partial}{\partial y} \right)^k g]_0 \right\} + O(h^{m+1}) \end{aligned}$$

Thus, putting  $G_1(h)$  as

$$(1.3.9) \quad G_1(h) = \sum_{r=0}^{m-1} \left( \sum_{j=1}^q \frac{\tau_{1j} \kappa_{jr}}{r!} \right) h^{r+1}$$

and noting that  $G_1(h)$  is of the order  $h$  and  $G_1(0)=0$ , we have the equation

$$\sum_{\ell=0}^m \frac{\kappa_{1\ell}}{\ell!} h^\ell = \sum_{\ell=0}^m \frac{h^\ell}{\ell!} \left\{ \sum_{k=0}^{\ell} \binom{\ell}{k} \rho_1^{\ell-k} (G_1(h))^k [D_0^{\ell-k} \left( \frac{\partial}{\partial y} \right)^k g]_0 \right\},$$

which is similar to (1.2.4). Hence, following after the proof of Theorem 1, we have

$$\kappa_{1\ell} = \rho_1^\ell [D_0^\ell g]_0 + \sum_{s=1}^{\ell-1} \binom{\ell}{s} \left\{ \sum_{t=1}^{m(\ell,s)} \frac{(\ell-s)!}{(\ell-s-t)!} \rho_1^{\ell-s-t} B_{s,t}(G_1'(0), \dots, G_1^{(s)}(0)) \right. \\ \left. \times [D_0^{\ell-s-t} (\frac{\partial}{\partial y})^t g]_0 \right\}$$

From (9), for  $k=1, 2, \dots, s$

$$G_1^{(k)}(h) = \sum_{r=k-1}^{m-1} \frac{(r+1)!}{(r-k+1)!} \left( \sum_j \frac{\tau_{1j} \kappa_{j,r}}{r!} \right) h^{r-k+1}$$

holds, which implies

$$G_1^{(k)}(0) = k! \left( \sum_j \frac{\tau_{1j} \kappa_{j,k-1}}{(k-1)!} \right) = k \sum_j \tau_{1j} \kappa_{j,k-1}$$

Thus we have the desired result.  $\square$

By Theorem 3,  $\kappa_{1\ell}$  is given as follows:

$$\kappa_{11} = \rho_1 [D_0 g]_0,$$

$$\kappa_{12} = \rho_1^2 [D_0^2 g]_0 + 2! B_{1,1} \left( \sum_j \tau_{1j} \kappa_{j0} \right) g_{y,0}$$

$$= \rho_1^2 [D_0^2 g]_0 + 2 \left( \sum_j \tau_{1j} \right) g_0 g_{y,0},$$

$$\kappa_{13} = \rho_1^3 [D_0^3 g]_0 + 3! \rho_1 B_{1,1} \left( \sum_j \tau_{1j} \kappa_{j0} \right) [D_0 g_y]_0 + 3 B_{2,1} \left( \sum_j \tau_{1j} \kappa_{j0}, 2 \sum_j \tau_{1j} \kappa_{j1} \right) g_y$$

$$= \rho_1^3 [D_0^3 g]_0 + 6 \rho_1 \left( \sum_j \tau_{1j} \right) g_0 [D_0 g_y]_0 + 6 \left( \sum_j \tau_{1j} \rho_j \right) [D_0 g]_0 g_{y,0}$$

The result with the help of REDUCE-2 is shown in Table 2

Here we employ the notation

$$T_{ik} = \sum_{j=1}^q \rho_j^k r_{ij} \quad , \quad i = 1, 2, \dots, q, \quad k = 0, 1, 2, \dots$$

From (6) and (7), the Taylor series expansion for  $y_1$  is given by

$$\begin{aligned} (1.3.10) \quad y_1 &= y_0 + hf_0 + \sum_{i=1}^q v_i h^2 \left( \sum_{\ell=0}^m \frac{\kappa_{i\ell}}{\ell!} h^\ell \right) + O(h^{m+3}) \\ &= y_0 + hf_0 + \sum_{\ell=0}^m \left( \sum_{i=1}^q v_i \kappa_{i\ell} \right) \frac{h^{\ell+2}}{\ell!} + O(h^{m+3}) \\ &= y_0 + hf_0 + \sum_{r=2}^m \left( \sum_{i=1}^q v_i \kappa_{i,r-2} \right) \frac{h^r}{(r-2)!} + O(h^{m+1}) \end{aligned}$$

On the other hand, from (1.2 2), the (second type) Taylor series expansion of the solution  $y(x_0+h)$  is given by

$$(1.3.11) \quad y(x_0+h) = y_0 + hf_0 + \sum_{r=2}^m \frac{\kappa_{r-2}}{r!} h^r + O(h^{m+1}),$$

where  $\kappa_\ell$  is represented by (1.2 5). The comparison of (10) and (11) brings the determining equation of the implicit (1,q)-stage formula, for which we have the following

**Theorem 4** Each  $\kappa_{i\ell}$  in (10) is constructed with the all elementary differentials included in the corresponding  $\kappa_\ell$  in (11). Hence the determining equation of the implicit



(1,q)-stage formula is of the form such as

(an integer)  $\times$  (a polynomial of  $v_i, \rho_i, \tau_{ij}$ ) = (an integer).

Proof From (10) and (11),  $\kappa_\ell$  and  $\kappa_{i,\ell}$  must satisfy

$$\frac{1}{\ell!} \sum_{i=1}^q v_i \kappa_{i\ell} = \frac{\kappa_\ell}{(\ell+2)!}, \quad \ell = 0, 1, 2, \dots, m-2,$$

which implies

$$(\ell+1)(\ell+2) \sum_{i=1}^q v_i \kappa_{i\ell} = \kappa_\ell$$

From (1.2.5) and (1.3.8) the conclusion follows  $\square$

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Table 2

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#### §1.4 Determining Equation for (1,q)-Stage Formula.

An algebraic computation according to Theorem 1 gives the number of elementary differentials including in each  $\kappa_\ell$ . Let  $m_\ell$  be the number of elementary differentials in  $\kappa_\ell$  and define the integer  $M_\ell$  by

$$M_\ell = \sum_{j=0}^{\ell} m_j$$

Each  $m_\ell$  and  $M_\ell$  are given in Table 3 up to  $\ell = 8$ .

Thus, we have  $M_\ell$  restrictions for the parameters  $v_i$ ,  $\rho_i$ ,  $r_{ij}$  of the formula. In the implicit (1,q)-stage formula the number of the parameters to be determined, say  $N_q^{(I)}$ , can be given as a simple function of  $q$

$$N_q^{(I)} = q(q+2)$$

It implies that the implicit (1,q)-stage formula can attain at least the order  $(\bar{\ell}+2)$  where  $\bar{\ell}$  is the largest integer satisfying the inequality  $M_{\bar{\ell}} \leq N_q^{(I)}$ . These relations are shown in Table 4

However, the above argument based on merely counting the number of the equations that must be satisfied, ignores the relationship between them. In fact, it may happen that  $M_\ell$  restrictions are satisfied with fewer than  $M_\ell$  variables. But, since we are interested in the explicit formula rather than implicit one, we shall not come into more investigation

for the attainable order of the implicit formula.

An explicit  $(1,q)$ -stage formula, which is defined by the parameters  $v_i$ ,  $\rho_i$  and  $\tau_{ij}$  ( $\tau_{ij} = 0$  for  $j \geq i$ ) in (1.3.6), has  $N_q^{(E)}$  parameters to be determined. Here  $N_q^{(E)}$  is given by

$$N_q^{(E)} = q(q+3)/2.$$

Hence, similar consideration for the implicit case gives the largest integer  $\ell^*$  satisfying the inequality  $M_\ell \leq N_q^{(E)}$ . Table 4 includes the relations between  $q$ , the number of stages, and  $\ell^*$

Table 3.

$\ell$	$m_\ell$	$M_\ell$
0	1	1
1	1	2
2	2	4
3	3	7
4	6	13
5	9	22
6	17	39
7	26	65
8	46	111

Table 4.

$q$	$N_q^{(I)}$	$\bar{\ell}$	$N_q^{(E)}$	$\ell^*$
1	3	1	2	1
2	8	3	5	2
3	15	4	9	3
4	24	5	14	4
5	35	5	20	5
6	48	6	27	5
7	63	6	35	6
8	80	7	44	6
9	99	7	54	6
10	120	8	65	7

Shintani has given some explicit one-step methods utilizing the second derivative [12], whose formulation coincides with our explicit (1,q)-stage formula. He has determined the parameters for  $q = 1, 2, 3, 4$  and  $5$  which give the formula obtaining the order  $3, 4, 5, 6$  and  $7$  respectively. His results attain the orders that we have argued as the least number  $l^*$  for each stage formula. Hence, it is a question whether Shintani's results can be improved.

We shall consider the determining equation for the explicit (1,q)-stage formula. Tables 1 and 2 give the equation as follows. We employ the notation for summation symbol such that the upper limit of summation can not exceed the variable of the preceding summation symbols, i.e.  $\sum_i \dots (\sum_j \dots)$  means  $\sum_{i=1}^q \dots (\sum_{j=1}^{i-1} \dots)$ . Moreover, the symbol  $T_{ik}$  means

$$T_{1k} = 0 \quad \text{and} \quad T_{ik} = \sum_{j=1}^{i-1} \rho_i^k \tau_{ij}, \quad i = 2, 3, \dots, q.$$

Determining equations.

$$l = 0: \quad (E-0) \quad 2 \sum_i v_i = 1$$

$$l = 1: \quad (E-1) \quad 6 \sum_i v_i \rho_i = 1$$

$$l = 2: \quad (E-21) \quad 12 \sum_i v_i \rho_i^2 = 1$$

$$(E-22) \quad 24 \sum_i v_i T_{i0} = 1$$

$$l = 3: \quad (E-31) \quad 20 \sum_i v_i \rho_i^3 = 1$$

$$(E-32) \quad 120 \sum_i v_i T_{i1} = 1$$

$$(E-33) \quad 120 \sum_i v_i \rho_i T_{i0} = 3$$

$$l = 4: \quad (E-41) \quad 30 \sum_i v_i \rho_i^4 = 1$$

$$(E-42) \quad 360 \sum_i v_i T_{i2} = 1$$

$$(E-43) \quad 720 \sum_i v_i \rho_i T_{i1} = 4$$

$$(E-44) \quad 360 \sum_i v_i \rho_i^2 T_{i0} = 6$$

$$(E-45) \quad 720 \sum_i \sum_j v_i \tau_{ij} T_{j0} = 1$$

$$(E-46) \quad 360 \sum_i v_i T_{i0}^2 = 3$$

$$l = 5: \quad (E-51) \quad 42 \sum_i v_i \rho_i^5 = 1$$

$$(E-52) \quad 840 \sum_i v_i T_{i3} = 1$$

$$(E-53) \quad 2520 \sum_i v_i \rho_i T_{i2} = 5$$

$$(E-54) \quad 2520 \sum_i v_i \rho_i^2 T_{i1} = 10$$

$$(E-55) \quad 5040 \sum_i \sum_j v_i \tau_{ij} T_{j1} = 1$$

$$(E-56) \quad 840 \sum_i v_i \rho_i^3 T_{i0} = 10$$

$$(E-57) \quad 5040 \sum_i \sum_j v_i (\rho_i + \rho_j) \tau_{ij} T_{j0} = 8$$

$$(E-58) \quad 5040 \sum_i v_i T_{i0} T_{i1} = 10$$

$$(E-59) \quad 2520 \sum_i v_i \rho_i T_{i0}^2 = 15$$

$$l = 6: \quad (E-601) \quad 56 \sum_i v_i \rho_i^6 = 1$$

$$(E-602) \quad 1680 \sum_i v_i T_{i4} = 1$$

$$(E-603) \quad 6720 \sum_i v_i \rho_i T_{i3} = 6$$

$$(E-604) \quad 10080 \sum_i v_i \rho_i^2 T_{i2} = 15$$

$$(E-605) \quad 20160 \sum_i \sum_j v_i \tau_{ij} T_{j2} = 1$$

$$(E-606) \quad 6720 \sum_i v_i \rho_i^3 T_{i1} = 20$$

$$(E-607) \quad 40320 \sum_i \sum_j v_i (\rho_i + \rho_j) \tau_{ij} T_{j1} = 10$$

$$(E-608) \quad 20160 \sum_i v_i T_{i1}^2 = 10$$

$$(E-609) \quad 1680 \sum_i v_i \rho_i^4 T_{i0} = 15$$

$$(E-610) \quad 40320 \sum_i \sum_j v_i \rho_i \rho_j \tau_{ij} T_{j0} = 18$$

$$(E-611) \quad 20160 \sum_i \sum_j v_i (\rho_i^2 + \rho_j^2) \tau_{ij} T_{j0} = 21$$

$$(E-612) \quad 40320 \sum_i \sum_j \sum_k v_i \tau_{ij} \tau_{jk} T_{k0} = 1$$

$$(E-613) \quad 20160 \sum_i v_i T_{i0} T_{i2} = 15$$

$$(E-614) \quad 40320 \sum_i v_i \rho_i T_{i0} T_{i1} = 60$$

$$(E-615) \quad 10080 \sum_i v_i \rho_i^2 T_{i0}^2 = 45$$

$$(E-616) \quad 20160 \sum_i \sum_j v_i \tau_{ij} (T_{j0} + 2T_{i0}) T_{j0} = 18$$

$$(E-617) \quad 6720 \sum_i v_i T_{i0}^3 = 15$$

$$l = 7: \quad (E-701) \quad \frac{1}{11} 72 \sum_i v_i \rho_i^7 = 1$$

$$(E-702) \quad 3024 \sum_i v_i T_{i5} = 1$$



$$(E-703) \quad 15120 \sum_i v_i \rho_i T_{i4} = 7$$

$$(E-704) \quad 30240 \sum_i v_i \rho_i^2 T_{i3} = 21$$

$$(E-705) \quad 60480 \sum_i \sum_j v_i \tau_{ij} T_{j3} = 1$$

$$(E-706) \quad 30240 \sum_i v_i \rho_i^3 T_{i2} = 35$$

$$(E-707) \quad 181440 \sum_i \sum_j v_i (\rho_i + \rho_j) \tau_{ij} T_{j2} = 12$$

$$(E-708) \quad 15120 \sum_i v_i \rho_i^4 T_{i1} = 35$$

$$(E-709) \quad 362880 \sum_i \sum_j v_i \rho_i \rho_j \tau_{ij} T_{j1} = 28$$

$$(E-710) \quad 181440 \sum_i \sum_j v_i (\rho_i^2 + \rho_j^2) \tau_{ij} T_{j1} = 31$$

$$(E-711) \quad 362880 \sum_i \sum_j \sum_k v_i \tau_{ij} \tau_{jk} T_{k1} = 1$$

$$(E-712) \quad 181440 \sum_i v_i T_{i1} T_{i2} = 35$$

$$(E-713) \quad 181440 \sum_i v_i \rho_i T_{i1}^2 = 70$$

$$(E-714) \quad 3024 \sum_i v_i \rho_i^5 T_{i0} = 21$$

$$(E-715) \quad 181440 \sum_i \sum_j v_i \rho_i \rho_j (\rho_i + \rho_j) \tau_{ij} T_{j0} = 105$$

$$(E-716) \quad 60480 \sum_i \sum_j v_i (\rho_i^3 + \rho_j^3) \tau_{ij} T_{j0} = 45$$

$$(E-717) \quad 362880 \sum_i \sum_j \sum_k v_i (\rho_i + \rho_j + \rho_k) \tau_{ij} \tau_{jk} T_{k0} = 15$$

$$(E-718) \quad 60480 \sum_i v_i T_{i0} T_{i3} = 21$$

$$(E-719) \quad 181440 \sum_i v_i \rho_i T_{i0} T_{i2} = 105$$

$$(E-720) \quad 181440 \sum_i v_i \rho_i^2 T_{i0} T_{i1} = 210$$

$$(E-722) \quad 362880 \sum_i \sum_j v_i \tau_{ij} (T_{i0} T_{j1} + T_{j0} T_{j1} + T_{j0} T_{i1}) = 66$$

$$(E-723) \quad 30240 \sum_i v_i \rho_i^3 T_{i0}^2 = 105$$

$$(E-724) \quad 181440 \sum_i \sum_j v_i (2\rho_i T_{i0} + \rho_j T_{j0}) \tau_{ij} T_{j0} = 84$$

$$(E-725) \quad 181440 \sum_i \sum_j v_i (\rho_i T_{j0} + 2\rho_j T_{i0}) \tau_{ij} T_{j0} = 120$$

$$(E-726) \quad 181440 \sum_i v_i T_{i0}^2 T_{i1} = 105$$

$$(E-727) \quad 60480 \sum_i v_i \rho_i T_{i0}^3 = 105$$

$$\ell = 8: (E-801) \quad 90 \sum_i v_i \rho_i^8 = 1$$

$$(E-802) \quad 5040 \sum_i v_i T_{i6} = 1$$

$$(E-803) \quad 30240 \sum_i v_i \rho_i T_{i5} = 8$$

$$(E-804) \quad 75600 \sum_i v_i \rho_i^2 T_{i4} = 28$$

- (E-805)  $151200 \sum_i \sum_j v_i \tau_{ij} T_{j4} = 1$
- (E-806)  $100800 \sum_i v_i \rho_i^3 T_{i3} = 56$
- (E-807)  $604800 \sum_i \sum_j v_i (\rho_i + \rho_j) \tau_{ij} T_{j3} = 14$
- (E-808)  $75600 \sum_i v_i \rho_i^4 T_{i2} = 70$
- (E-809)  $1814400 \sum_i \sum_j v_i \rho_i \rho_j \tau_{ij} T_{j2} = 40$
- (E-810)  $907200 \sum_i \sum_j v_i (\rho_i^2 + \rho_j^2) \tau_{ij} T_{j2} = 43$
- (E-811)  $1814400 \sum_i \sum_j \sum_k v_i \tau_{ij} \tau_{jk} T_{k2} = 1$
- (E-812)  $453600 \sum_i v_i T_{i2}^2 = 35$
- (E-813)  $30240 \sum_i v_i \rho_i^5 T_{i1} = 56$
- (E-814)  $1814400 \sum_i \sum_j v_i \rho_i \rho_j (\rho_i + \rho_j) \tau_{ij} T_{j1} = 192$
- (E-815)  $604800 \sum_i \sum_j v_i (\rho_i^3 + \rho_j^3) \tau_{ij} T_{ji} = 76$
- (E-816)  $3628800 \sum_i \sum_j \sum_k v_i (\rho_i + \rho_j + \rho_k) \tau_{ij} \tau_{jk} T_{k1} = 18$
- (E-817)  $604800 \sum_i v_i T_{i1} T_{i3} = 56$
- (E-818)  $1814400 \sum_i v_i \rho_i T_{i1} T_{i2} = 280$

$$(E-819) \quad 907200 \sum_i v_i \rho_i^2 T_{i1}^2 = 280$$

$$(E-820) \quad 1814400 \sum_i \sum_j v_i \tau_{ij} T_{j1} (2T_{i1} + T_{j1}) = 66$$

$$(E-821) \quad 5040 \sum_i v_i \rho_i^6 T_{i0} = 28$$

$$(E-822) \quad 907200 \sum_i \sum_j v_i \rho_i^2 \rho_j^2 \tau_{ij} T_{j0} = 168$$

$$(E-823) \quad 604800 \sum_i \sum_j v_i \rho_i \rho_j (\rho_i^2 + \rho_j^2) \tau_{ij} T_{j0} = 248$$

$$(E-824) \quad 151200 \sum_i \sum_j v_i (\rho_i^4 + \rho_j^4) \tau_{ij} T_{j0} = 85$$

$$(E-825) \quad 3628800 \sum_i \sum_j \sum_k v_i (\rho_i \rho_j + \rho_j \rho_k + \rho_j \rho_k) \tau_{ij} \tau_{jk} T_{k0} = 82$$

$$(E-826) \quad 1814400 \sum_i \sum_j \sum_k v_i (\rho_i^2 + \rho_j^2 + \rho_k^2) \tau_{ij} \tau_{jk} T_{k0} = 49$$

$$(E-827) \quad 3628800 \sum_i \sum_j \sum_k \sum_l v_i \tau_{ij} \tau_{jk} \tau_{kl} T_{l0} = 1$$

$$(E-828) \quad 151200 \sum_i v_i T_{i0} T_{i4} = 28$$

$$(E-829) \quad 604800 \sum_i v_i \rho_i T_{i0} T_{i3} = 168$$

$$(E-830) \quad 907200 \sum_i v_i \rho_i^2 T_{i0} T_{i2} = 420$$

$$(E-831) \quad 1814400 \sum_i \sum_j v_i \tau_{ij} (T_{i2} T_{j0} + T_{i0} T_{j2} + T_{j0} T_{j2}) = 113$$

$$(E-832) \quad 604800 \sum_i v_i \rho_i^3 T_{i0} T_{i1} = 560$$

$$(E-833) \quad 3628800 \sum_i \sum_j v_i \tau_{ij} (\rho_j T_{i0} T_{j1} + \rho_j T_{i1} T_{j0} + \rho_i T_{j0} T_{j1}) = 360$$

$$(E-834) \quad 3628800 \sum_i \sum_j v_i \tau_{ij} (\rho_i T_{i0} T_{j1} + \rho_i T_{i1} T_{j0} + \rho_j T_{j0} T_{j1}) = 508$$

$$(E-835) \quad 1814400 \sum_i v_i T_{i0} T_{i1}^2 = 280$$

$$(E-836) \quad 75600 \sum_i v_i \rho_i^4 T_{i0}^2 = 210$$

$$(E-837) \quad 907200 \sum_i \sum_j v_i \tau_{ij} (\rho_i^2 T_{j0} + 2\rho_j^2 T_{i0}) T_{j0} = 252$$

$$(E-838) \quad 1814400 \sum_i \sum_j v_i \rho_i \rho_j \tau_{ij} (2T_{i0} + T_{j0}) T_{j0} = 624$$

$$(E-839) \quad 907200 \sum_i \sum_j v_i \tau_{ij} (\rho_j^2 T_{j0} + 2\rho_i^2 T_{i0}) T_{j0} = 465$$

$$(E-840) \quad 1814400 \sum_i \sum_j \sum_k v_i \tau_{ij} (2\tau_{jk} T_{i0} T_{k0} + 2\tau_{jk} T_{j0} T_{k0} + \tau_{ik} T_{j0} T_{k0} + \tau_{jk} T_{k0}^2) = 81$$

$$(E-841) \quad 907200 \sum_i v_i T_{i0}^2 T_{i2} = 210$$

$$(E-842) \quad 1814400 \sum_i v_i \rho_i T_{i0}^2 T_{i1} = 840$$

$$(E-843) \quad 302400 \sum_i v_i \rho_i^2 T_{i0}^3 = 420$$

$$(E-844) \quad 1814400 \sum_i \sum_j v_i \tau_{ij} T_{i0} T_{j0}^2 = 84$$

$$(E-845) \quad 604800 \sum_i \sum_j v_i \tau_{ij} (3T_{i0}^2 + T_{j0}^2) T_{j0} = 225$$

$$(E-846) \quad 151200 \sum_i v_i T_{i0}^4 = 105$$

## §1.5 Attainable Order of (1,1)- and (1,2)-Stage Formulas

The explicit (1,q)-stage formula is said to have the attainable order  $m$  if  $m$  is the largest integer for which

$$y(x+h) - y_1 = O(h^{m+1})$$

among all combinations of the parameters of the formula, where  $y(x)$  is the analytical solution and  $y_1$  is given by (1.3 6). The definition of the attainable order will be extended, if necessary, to general (p,q)-stage formula.

It is obvious that a (1,q)-stage formula has the attainable order  $m$  if and only if the determining equations corresponding up to  $l$  have at least one solution, but they have no solution up to  $l+1$ , where  $l = m-2$ .

**Theorem 5.** The attainable order of (1,1)-stage formula is 3

**Proof** The left-hand side of the equation (E-22) is equal to

$$24 \sum_i v_i (\sum_j r_{ij}),$$

which vanishes for (1,1)-stage formula because  $\sum_j r_{ij} = 0$ . This means that the parameters  $v_1$  and  $\rho_1$  can satisfy merely the equations (E-0) and (E-1)  $\square$

Theorem 6. The attainable order of (1,2)-stage formula is equal to 4.

Proof Assume that the formula attains order 5, that is, the parameters  $v_1, v_2, \rho_1, \rho_2$  and  $\tau_{21}$  satisfy the equations (E-0) ~ (E-33).

$$(1.5.1) \quad v_1 + v_2 = \frac{1}{2}$$

$$(1.5.2) \quad v_1 \rho_1 + v_2 \rho_2 = \frac{1}{6}$$

$$(1.5.3) \quad v_2 \tau_{21} = \frac{1}{24}$$

$$(1.5.4) \quad v_1 \rho_1^2 + v_2 \rho_2^2 = \frac{1}{12}$$

$$(1.5.5) \quad v_2 \rho_2 \tau_{21} = \frac{1}{40}$$

$$(1.5.6) \quad v_2 \rho_1 \tau_{21} = \frac{1}{120}$$

$$(1.5.7) \quad v_1 \rho_1^3 + v_2 \rho_2^3 = \frac{1}{20}$$

The equations (1), (2) and (4) yield a matrix equation

$$\begin{bmatrix} 1 & 1 & 1/2 \\ \rho_1 & \rho_2 & 1/6 \\ \rho_1^2 & \rho_2^2 & 1/12 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ -1 \end{bmatrix} = 0,$$

which implies

$$(1.5.8) \quad \begin{vmatrix} 1 & 1 & 1/2 \\ \rho_1 & \rho_2 & 1/6 \\ \rho_1^2 & \rho_2^2 & 1/12 \end{vmatrix} = 0$$

for the existence of nontrivial solution  $[v_1, v_2, -1]^t$

On the other hand, (3), (5) and (6) give the values

$$\rho_1 = \frac{1}{5}, \quad \rho_2 = \frac{3}{5},$$

which specify the determinant of (8) by  $\frac{1}{250}$ . This contradiction implies the statement  $\square$

Note. Shintani gives (1,1)-stage formula with parameters  $v_1 = \frac{1}{2}$  and  $\rho_1 = \frac{1}{3}$ . He also gives (1,2)-stage formula with  $v_1 = (9+\sqrt{6})/36$ ,  $v_2 = (9-\sqrt{6})/36$ ,  $\rho_1 = (4-\sqrt{6})/10$ ,  $\rho_2 = (4+\sqrt{6})/10$ ,  $\tau_{21} = (9+\sqrt{6})/50$ . These parameters are not unique solution (1.5 1) ~ (1.5 4). The solution of them is represented with one parameter  $\rho$  by the following:

$$\begin{aligned} \rho_1 &= \rho & (\rho \neq \frac{1}{3}), \\ \rho_2 &= (2\rho-1)/2(3\rho-1), \\ v_1 &= 1/6(6\rho^2+1), \\ v_2 &= (9\rho^2+1)/3(6\rho^2+1), \\ \tau_{21} &= (6\rho^2+1)/8(9\rho^2+1) \end{aligned}$$



# §1 6 Attainable Order of (1,3)-Stage Formula.

The determining equation for the explicit (1,3)-stage formula are given as follows:

$$(E-0) \quad v_1 + v_2 + v_3 = \frac{1}{2}$$

$$(E-1) \quad v_1 \rho_1 + v_2 \rho_2 + v_3 \rho_3 = \frac{1}{6}$$

$$(E-21) \quad v_1 \rho_1^2 + v_2 \rho_2^2 + v_3 \rho_3^2 = \frac{1}{12}$$

$$(E-22) \quad v_2 \tau_{21} + v_3 (\tau_{31} + \tau_{32}) = \frac{1}{24}$$

$$(E-31) \quad v_1 \rho_1^3 + v_2 \rho_2^3 + v_3 \rho_3^3 = \frac{1}{20}$$

$$(E-32) \quad v_2 \rho_2 \tau_{21} + v_3 \rho_3 (\tau_{31} + \tau_{32}) = \frac{1}{40}$$

$$(E-33) \quad v_2 \rho_1 \tau_{21} + v_3 (\rho_1 \tau_{31} + \rho_2 \tau_{32}) = \frac{1}{120}$$

$$(E-41) \quad v_1 \rho_1^4 + v_2 \rho_2^4 + v_3 \rho_3^4 = \frac{1}{30}$$

$$(E-42) \quad v_2 \rho_2^2 \tau_{21} + v_3 \rho_3^2 (\tau_{31} + \tau_{32}) = \frac{1}{60}$$

$$(E-43) \quad v_2 \rho_2 \rho_1 \tau_{21} + v_3 \rho_3 (\rho_1 \tau_{31} + \rho_2 \tau_{32}) = \frac{1}{180}$$

$$(E-44) \quad v_2 \rho_1^2 \tau_{21} + v_3 (\rho_1^2 \tau_{31} + \rho_2^2 \tau_{32}) = \frac{1}{360}$$

$$(E-45) \quad v_2 \tau_{21}^2 + v_3 (\tau_{31} + \tau_{32})^2 = \frac{1}{120}$$

$$(E-46) \quad v_3 \tau_{21} \tau_{32} = \frac{1}{720}$$

It is remarkable that none of the factors on the left of (E-46) can vanish.

Assume that two of  $\rho_1, \rho_2, \rho_3$  are equal, say  $\rho_I = \rho_J$ . Then, from (E-0), (E-1), (E-21), (E-31) and (E-41), we see that

$$\begin{bmatrix} 1 & 1 & \frac{1}{2} \\ \rho_I & \rho_K & \frac{1}{6} \\ \rho_I^2 & \rho_K^2 & \frac{1}{12} \end{bmatrix} \begin{bmatrix} v_I + v_J \\ v_K \\ -1 \end{bmatrix} = 0 ,$$

$$\begin{bmatrix} 1 & 1 & \frac{1}{6} \\ \rho_I & \rho_K & \frac{1}{12} \\ \rho_I^2 & \rho_K^2 & \frac{1}{20} \end{bmatrix} \begin{bmatrix} \rho_I (v_I + v_J) \\ \rho_K v_K \\ -1 \end{bmatrix} = 0 ,$$

$$\begin{bmatrix} 1 & 1 & \frac{1}{12} \\ \rho_I & \rho_K & \frac{1}{20} \\ \rho_I^2 & \rho_K^2 & \frac{1}{30} \end{bmatrix} \begin{bmatrix} \rho_I^2 (v_I + v_J) \\ \rho_K^2 v_K \\ -1 \end{bmatrix} = 0$$

The condition that the above three equations have non-trivial solutions, implies the equations with respect to  $\rho_I, \rho_K$  as follows:

$$(\rho_K - \rho_I) \left\{ \frac{1}{2} \rho_I \rho_K - \frac{1}{6} (\rho_I + \rho_K) + \frac{1}{12} \right\} = 0,$$

$$(\rho_K - \rho_I) \left\{ \frac{1}{6} \rho_I \rho_K - \frac{1}{12} (\rho_I + \rho_K) + \frac{1}{20} \right\} = 0$$

and

$$(\rho_K - \rho_I) \left\{ \frac{1}{12} \rho_I \rho_K - \frac{1}{20} (\rho_I + \rho_K) + \frac{1}{30} \right\} = 0$$

If  $\rho_I \neq \rho_K$ ,  $\rho_I$  and  $\rho_K$  must satisfy the equations

$$\frac{1}{2} \rho_I \rho_K - \frac{1}{6} (\rho_I + \rho_K) + \frac{1}{12} = \frac{1}{6} \rho_I \rho_K - \frac{1}{12} (\rho_I + \rho_K) + \frac{1}{20} = \frac{1}{12} \rho_I \rho_K - \frac{1}{20} (\rho_I + \rho_K) + \frac{1}{30} = 0,$$

which is impossible. The case of  $\rho_1 = \rho_2 = \rho_3$  leads to a contradiction because of

$$v_1 + v_2 + v_3 = \frac{1}{2},$$

$$\rho_1 (v_1 + v_2 + v_3) = \frac{1}{6},$$

$$\rho_1^2 (v_1 + v_2 + v_3) = \frac{1}{12},$$

induced by (E-0), (E-1), (E-21), respectively

Hence no two of  $\rho_1, \rho_2, \rho_3$  are equal. It is convenient to define

$$A_i = \sum_{j=1}^{i-1} \tau_{ij} - \frac{1}{2} \rho_i^2 \quad (i=1,2,3)$$

Since we consider the explicit formula,  $A_1 = -\frac{1}{2}\rho_1^2$  holds.

Then, we have simultaneous linear equations

$$\begin{bmatrix} 1 & 1 & 1 \\ \rho_1 & \rho_2 & \rho_3 \\ \rho_1^2 & \rho_2^2 & \rho_3^2 \end{bmatrix} \begin{bmatrix} v_1 A_1 \\ v_2 A_2 \\ v_3 A_3 \end{bmatrix} = 0$$

by (E-21), (E-22), (E-31), (E-32), (E-41) and (E-42). Since no two of  $\rho_1, \rho_2, \rho_3$  are equal, all of  $v_1 A_1, v_2 A_2, v_3 A_3$  vanish. By virtue of the above mentioned remark, we distinguish the following four cases

Case 1.  $A_1 = A_2 = A_3 = 0$

The equations  $A_1=0$  and  $A_2=0$  imply  $\rho_1=0$  and  $\tau_{21}=\frac{1}{2}\rho_2^2$ . Then, (E-43) and (E-44) bring the equations  $v_3 \rho_2 \rho_3 \tau_{32} = \frac{1}{180}$  and  $v_3 \rho_2^2 \tau_{32} = \frac{1}{360}$ , which give the identity  $\rho_3 = 2\rho_2$

Thus (E-1), (E-21) and (E-31) imply the equation

$$\begin{bmatrix} \rho_2 & 2\rho_2 & \frac{1}{6} \\ \rho_2^2 & 4\rho_2^2 & \frac{1}{12} \\ \rho_3^3 & 8\rho_3^3 & \frac{1}{20} \end{bmatrix} \begin{bmatrix} v_2 \\ v_3 \\ -1 \end{bmatrix} = 0,$$

which yields a quadratic equation of  $\rho_2$

$$20\rho_2^2 - 15\rho_2 + 3 = 0$$

because of  $\rho_2 \neq 0$ . But the above quadratic equation has no real roots

Case 2.  $v_1=0$  and  $A_2 = A_3 = 0$ .

In such case, we have the equations

$$\tau_{21} = \frac{1}{2} \rho_2^2$$

and

$$\tau_{31} + \tau_{32} = \frac{1}{2} \rho_3^2 .$$

Substitution of  $\tau_{21} = \frac{1}{2} \rho_2^2$  and  $\tau_{31} = \frac{1}{2} \rho_3^2 - \tau_{32}$  into (E-44) implies

$$\rho_1^2 + 24v_3\tau_{32}(\rho_2^2 - \rho_1^2) = \frac{1}{15}$$

Employing the equation

$$(*) \quad v_3\rho_2^2\tau_{32} = \frac{1}{360}$$

induced by (E-46), we obtain

$$\rho_1(1 - 24v_3\tau_{32}) = 0$$

Hence, the equation  $\rho_1=0$  or  $v_3\tau_{32}=\frac{1}{24}$  holds. The case of  $\rho_1=0$  is equivalent to Case 1. The equation  $v_3\tau_{32}=\frac{1}{24}$  yields

$$\rho_1 + 24v_3\tau_{32}(\rho_2 - \rho_1) = \rho_2 = \frac{1}{5}$$

by (E-33) The equation (\*), however, implies  $\rho_2^2=\frac{1}{15}$ , which leads to a contradiction

Case 3.  $v_2 = 0$  and  $A_1 = A_3 = 0$

$A_1 = 0$  implies  $\rho_1 = 0$ . Then, (E-1) and (E-21) bring the equations

$$v_3 \rho_3 = \frac{1}{6}$$

and

$$v_3 \rho_3^2 = \frac{1}{12}.$$

Hence we see  $\rho_3 = \frac{1}{2}$  and  $v_3 = \frac{1}{3}$ . It contradicts the equation  $v_3 \rho_3^3 = \frac{1}{20}$  induced by (E-31)

Case 4.  $v_1 = 0$ ,  $v_2 = 0$  and  $A_3 = 0$ .

The equations (E-0) and (E-1) yield  $v_3 = \frac{1}{2}$  and  $\rho_3 = \frac{1}{3}$ .

Again, it contradicts the equation  $v_3 \rho_3^3 = \frac{1}{20}$  induced by (E-31).

Thus, we can conclude that the determining equations (E-0) ~ (E-46) have no solutions. The proof of the following theorem is now accomplished.

**Theorem 7** The explicit (1,3)-stage formula can not attain order 6 Its attainable order is 5.

Note. Shintani gives (1,3)-stage formula with parameters

$$v_1 = \frac{1}{12}, v_2 = (5+\sqrt{5})/24, v_3 = (5-\sqrt{5})/24, \rho_1 = 0, \rho_2 = (5-\sqrt{5})/10.$$

$$\tau_{21} = (3-\sqrt{5})/20, \quad \rho_3 = (5+\sqrt{5})/10, \quad \tau_{31} = 0 \quad \text{and} \quad \tau_{32} = (3+\sqrt{5})/20$$

These parameters are also not unique solution of (E-0)~(E-33).



### §1.7 Attainable Order of (1,4)-Stage Formula.

The determining equation for the explicit (1,4)-stage formula are given by the following:

$$(E-0) \quad v_1 + v_2 + v_3 + v_4 = \frac{1}{2}$$

$$(E-1) \quad v_1 \rho_1 + v_2 \rho_2 + v_3 \rho_3 + v_4 \rho_4 = \frac{1}{6}$$

$$(E-21) \quad v_1 \rho_1^2 + v_2 \rho_2^2 + v_3 \rho_3^2 + v_4 \rho_4^2 = \frac{1}{12}$$

$$(E-22) \quad v_2 \tau_{21} + v_3 (\tau_{31} + \tau_{32}) + v_4 (\tau_{41} + \tau_{42} + \tau_{43}) = \frac{1}{24}$$

$$(E-31) \quad v_1 \rho_1^3 + v_2 \rho_2^3 + v_3 \rho_3^3 + v_4 \rho_4^3 = \frac{1}{20}$$

$$(E-32) \quad v_2 \rho_2 \tau_{21} + v_3 \rho_3 (\tau_{31} + \tau_{32}) + v_4 \rho_4 (\tau_{41} + \tau_{42} + \tau_{43}) = \frac{1}{40}$$

$$(E-33) \quad v_2 \rho_1 \tau_{21} + v_3 (\rho_1 \tau_{31} + \rho_2 \tau_{32}) + v_4 (\rho_1 \tau_{41} + \rho_2 \tau_{42} + \rho_3 \tau_{43}) = \frac{1}{120}$$

$$(E-41) \quad v_1 \rho_1^4 + v_2 \rho_2^4 + v_3 \rho_3^4 + v_4 \rho_4^4 = \frac{1}{30}$$

$$(E-42) \quad v_2 \rho_2^2 \tau_{21} + v_3 \rho_3^2 (\tau_{31} + \tau_{32}) + v_4 \rho_4^2 (\tau_{41} + \tau_{42} + \tau_{43}) = \frac{1}{60}$$

$$(E-43) \quad v_2 \rho_2 \rho_1 \tau_{21} + v_3 \rho_3 (\rho_1 \tau_{31} + \rho_2 \tau_{32}) + v_4 \rho_4 (\rho_1 \tau_{41} + \rho_2 \tau_{42} + \rho_3 \tau_{43}) = \frac{1}{180}$$

$$(E-44) \quad v_2 \rho_1^2 \tau_{21} + v_3 (\rho_1^2 \tau_{31} + \rho_2^2 \tau_{32}) + v_4 (\rho_1^2 \tau_{41} + \rho_2^2 \tau_{42} + \rho_3^2 \tau_{43}) = \frac{1}{360}$$

$$(E-45) \quad v_3 \tau_{21} \tau_{32} + v_4 (\tau_{21} \tau_{42} + \tau_{31} \tau_{43} + \tau_{32} \tau_{43}) = \frac{1}{720}$$

$$(E-46) \quad v_2 \tau_{21}^2 + v_3 (\tau_{31} + \tau_{32})^2 + v_4 (\tau_{41} + \tau_{42} + \tau_{43})^2 = \frac{1}{120}$$

$$(E-51) \quad v_1 \rho_1^5 + v_2 \rho_2^5 + v_3 \rho_3^5 + v_4 \rho_4^5 = \frac{1}{42}$$

$$(E-52) \quad v_2 \rho_2^3 \tau_{21} + v_3 \rho_3^3 (\tau_{31} + \tau_{32}) + v_4 \rho_4^3 (\tau_{41} + \tau_{42} + \tau_{43}) = \frac{1}{84}$$

$$(E-53) \quad v_2 \rho_2^2 \rho_1 \tau_{21} + v_3 \rho_3^2 (\rho_1 \tau_{31} + \rho_2 \tau_{32}) + v_4 \rho_4^2 (\rho_1 \tau_{41} + \rho_2 \tau_{42} + \rho_3 \tau_{43}) = \frac{1}{252}$$

$$(E-54) \quad v_2 \rho_2 \rho_1^2 \tau_{21} + v_3 \rho_3 (\rho_1^2 \tau_{31} + \rho_2^2 \tau_{32}) + v_4 \rho_4 (\rho_1^2 \tau_{41} + \rho_2^2 \tau_{42} + \rho_3^2 \tau_{43}) = \frac{1}{504}$$

$$(E-55) \quad v_2 \rho_1^3 \tau_{21} + v_3 (\rho_1^3 \tau_{31} + \rho_2^3 \tau_{32}) + v_4 (\rho_1^3 \tau_{41} + \rho_2^3 \tau_{42} + \rho_3^3 \tau_{43}) = \frac{1}{840}$$

$$(E-56) \quad v_3 (\rho_2 + \rho_3) \tau_{21} \tau_{32} + v_4 (\rho_2 + \rho_4) \tau_{21} \tau_{42} + v_4 (\rho_3 + \rho_4) (\tau_{31} \tau_{43} + \tau_{32} \tau_{43}) = \frac{1}{630}$$

$$(E-57) \quad v_3 \rho_1 \tau_{21} \tau_{32} + v_4 \rho_1 (\tau_{21} \tau_{42} + \tau_{31} \tau_{43}) + v_4 \rho_2 \tau_{32} \tau_{43} = \frac{1}{5040}$$

$$(E-58) \quad v_2 \rho_1 \tau_{21}^2 + v_3 (\rho_1 \tau_{31}^2 + \rho_1 \tau_{31} \tau_{32} + \rho_2 \tau_{31} \tau_{32} + \rho_2 \tau_{32}^2) + v_4 (\rho_1 \tau_{41}^2 + \rho_2 \tau_{42}^2 + \rho_3 \tau_{43}^2) \\ + v_4 \rho_1 (\tau_{41} \tau_{42} + \tau_{41} \tau_{43}) + v_4 \rho_2 (\tau_{41} \tau_{42} + \tau_{42} \tau_{43}) + v_4 \rho_3 (\tau_{31} \tau_{43} + \tau_{42} \tau_{43}) \\ = \frac{1}{504}$$

$$(E-59) \quad v_2 \rho_2 \tau_{21}^2 + v_3 \rho_3 (\tau_{31} + \tau_{32})^2 + v_4 \rho_4 (\tau_{41} + \tau_{42} + \tau_{43})^2 = \frac{1}{168}$$

The question is whether any parameters  $v_i$ ,  $\rho_i$  and  $\tau_{ij}$  exist to satisfy these 22 equations simultaneously. It is helpful for investigation to introduce the following notations:

$$T_{i0} = \sum_{j=1}^{i-1} \tau_{ij}, \quad T_{i1} = \sum_{j=1}^{i-1} \rho_j \tau_{ij} \quad (i=1,2,3,4)$$

( $T_{10}$  and  $T_{11}$  mean zero.)

$$A_i = T_{i0} - \frac{1}{2}\rho_i^2, \quad B_i = T_{i1} - \frac{1}{6}\rho_i^3 \quad (i=1,2,3,4).$$

Then, from (E-21), (E-22), (E-31), (E-32), (E-33), (E-41), (E-42), (E-43), (E-51), (E-52) and (E-53), we easily see that

$$(1.7.1) \quad \sum_i v_i A_i = \sum_i v_i \rho_i A_i = \sum_i v_i \rho_i^2 A_i = \sum_i v_i \rho_i^3 A_i = 0$$

and

$$(1.7.2) \quad \sum_i v_i B_i = \sum_i v_i \rho_i B_i = \sum_i v_i \rho_i^2 B_i = 0.$$

The equations (1) means

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ \rho_1 & \rho_2 & \rho_3 & \rho_4 \\ \rho_1^2 & \rho_2^2 & \rho_3^2 & \rho_4^2 \\ \rho_1^3 & \rho_2^3 & \rho_3^3 & \rho_4^3 \end{pmatrix} \begin{pmatrix} v_1 A_1 \\ v_2 A_2 \\ v_3 A_3 \\ v_4 A_4 \end{pmatrix} = 0$$

We now distinguish two cases according as two of  $\rho_1, \rho_2, \rho_3, \rho_4$  are equal or otherwise

Case 1. Two of  $\rho_1, \rho_2, \rho_3, \rho_4$  are equal

Assume that two of them are equal, say  $\rho_I = \rho_J$   
 Equations (E-0), (E-1), (E-21), (E-31), (E-41) and (E-51)  
 give three simultaneous linear equations as follows:

$$\begin{bmatrix} 1 & 1 & 1 & \frac{1}{2} \\ \rho_I & \rho_K & \rho_L & \frac{1}{6} \\ \rho_I^2 & \rho_K^2 & \rho_L^2 & \frac{1}{12} \\ \rho_I^3 & \rho_K^3 & \rho_L^3 & \frac{1}{20} \end{bmatrix} \begin{bmatrix} v_I + v_J \\ v_K \\ v_L \\ -1 \end{bmatrix} = 0,$$

$$\begin{bmatrix} 1 & 1 & 1 & \frac{1}{6} \\ \rho_I & \rho_K & \rho_L & \frac{1}{12} \\ \rho_I^2 & \rho_K^2 & \rho_L^2 & \frac{1}{20} \\ \rho_I^3 & \rho_K^3 & \rho_L^3 & \frac{1}{30} \end{bmatrix} \begin{bmatrix} \rho_I(v_I + v_K) \\ \rho_K v_K \\ \rho_L v_K \\ -1 \end{bmatrix} = 0,$$

$$\begin{bmatrix} 1 & 1 & 1 & \frac{1}{12} \\ \rho_I & \rho_K & \rho_L & \frac{1}{20} \\ \rho_I^2 & \rho_K^2 & \rho_L^2 & \frac{1}{30} \\ \rho_I^3 & \rho_K^3 & \rho_L^3 & \frac{1}{42} \end{bmatrix} \begin{bmatrix} \rho_I^2(v_I + v_J) \\ \rho_K^2 v_K \\ \rho_L^2 v_L \\ -1 \end{bmatrix} = 0$$

The condition that these equations have non-trivial solutions,  
 implies the determinants of matrices to be vanishing. Hence,  
 we see that the equations

$$\frac{1}{60}(\rho_I - \rho_K)(\rho_K - \rho_L)(\rho_L - \rho_I)\{-30\rho_I\rho_K\rho_L + 10(\rho_I\rho_K + \rho_K\rho_L + \rho_L\rho_I) \\ - 5(\rho_I + \rho_K + \rho_L) + 3\} = 0,$$

$$\frac{1}{60}(\rho_I - \rho_K)(\rho_K - \rho_L)(\rho_L - \rho_I)\{-10\rho_I\rho_K\rho_L + 5(\rho_I\rho_K + \rho_K\rho_L + \rho_L\rho_I) \\ - 3(\rho_I + \rho_K + \rho_L) + 2\} = 0$$

and

$$\frac{1}{420}(\rho_I - \rho_K)(\rho_K - \rho_L)(\rho_L - \rho_I)\{-35\rho_I\rho_K\rho_L + 21(\rho_I\rho_K + \rho_K\rho_L + \rho_L\rho_I) \\ - 14(\rho_I + \rho_K + \rho_L) + 10\} = 0$$

hold. We can distinguish three cases.

- (i) At least three of  $\rho_i$  are equal.
- (ii)  $\rho_I = \rho_J$  and  $\rho_K = \rho_L$
- (iii)  $\rho_I, \rho_K, \rho_L$  are distinct, and the above equations hold.

But, the case (i) can not hold by the similar reason mentioned at the first part of §1.6. In the case (ii), (E-0), (E-1), (E-21), (E-31) and (E-41) imply the equations

$$\begin{bmatrix} 1 & 1 & \frac{1}{2} \\ \rho_I & \rho_K & \frac{1}{6} \\ \rho_I^2 & \rho_K^2 & \frac{1}{12} \end{bmatrix} \begin{bmatrix} v_I + v_J \\ v_K + v_L \\ -1 \end{bmatrix} = 0,$$

$$\begin{pmatrix} 1 & 1 & \frac{1}{6} \\ \rho_I & \rho_K & \frac{1}{12} \\ \rho_I^2 & \rho_K^2 & \frac{1}{20} \end{pmatrix} \begin{pmatrix} \rho_I(v_I+v_J) \\ \rho_K(v_K+v_L) \\ -1 \end{pmatrix} = 0,$$

$$\begin{pmatrix} 1 & 1 & \frac{1}{12} \\ \rho_I & \rho_K & \frac{1}{20} \\ \rho_I^2 & \rho_K^2 & \frac{1}{30} \end{pmatrix} \begin{pmatrix} \rho_I^2(v_I+v_J) \\ \rho_K^2(v_K+v_L) \\ -1 \end{pmatrix} = 0$$

Thus, by the same reason as for case (i), these equations lead to a contradiction.

In the case (iii), we easily see the equations

$$\rho_I + \rho_K + \rho_L = \frac{9}{7},$$

$$\rho_I \rho_K + \rho_K \rho_L + \rho_L \rho_I = \frac{3}{7}$$

and

$$\rho_I \rho_K \rho_L = \frac{1}{35},$$

which imply that  $\rho_I, \rho_K, \rho_L$  are distinct roots of the cubic equation

$$(1.7.3) \quad x^3 - \frac{9}{7}x^2 + \frac{3}{7}x - \frac{1}{35} = 0$$

The cubic equation is irreducible and has three distinct real roots given as follows:

Let  $\theta$  be an angle such that

$$(1.7 \ 4) \quad \cos 3\theta = \frac{1}{5\sqrt{2}} \quad (0 < 3\theta \leq \frac{\pi}{2}).$$

Then, the roots are

$$(1.7 \ 5) \quad \begin{cases} R_0 = \frac{1}{7}(3+2\sqrt{2} \cos\theta), \\ R_1 = \frac{1}{7}(3-\sqrt{2} \cos\theta + \sqrt{6} \sin\theta), \\ R_{-1} = \frac{1}{7}(3-\sqrt{2} \cos\theta - \sqrt{6} \sin\theta) \end{cases}$$

Some algebraic properties on the equation (3) are the followings:

Lemma 1 7.1. The roots  $R_0, R_1, R_{-1}$  are equal to none of  $0, \frac{1}{7}, \frac{1}{3}$ .

Proof Substitution of  $0, \frac{1}{7}$  and  $\frac{1}{3}$  into the cubic polynomial of (3) gives  $-\frac{1}{35}, \frac{16}{1715}$  and  $\frac{8}{945}$ , respectively  $\square$

Lemma 1 7.2 The equation (3) has no common roots with the cubic equation

$$(1 \ 7 \ 6) \quad x^3 - \frac{3}{8}x^2 - \frac{3}{16}x + \frac{3}{64} = 0$$

Proof Put

$$f_1(x) = x^3 - \frac{9}{7}x^2 + \frac{3}{7}x - \frac{1}{35}$$

and

$$f_2(x) = x^3 - \frac{3}{8}x^2 - \frac{3}{16}x + \frac{3}{64}.$$

The Sylvester's determinant  $D(f_1, f_2)$  is equal to  $-3437/32768000$ .  $\square$

Lemma 1.7.3. The equation (3) has no roots, one of which is the triple of another.

Proof Assume that one of roots is equal to the triple of another, then the root satisfy another cubic equation

$$27x^3 - \frac{81}{7}x^2 + \frac{9}{7}x - \frac{1}{35} = 0.$$

That is,

$$x^3 - \frac{3}{7}x^2 + \frac{1}{21}x - \frac{1}{945} = 0$$

Put

$$f_1(x) = x^3 - \frac{3}{7}x^2 + \frac{1}{21}x - \frac{1}{945}$$

and

$$f_2(x) = x^3 - \frac{3}{7}x^2 + \frac{1}{21}x - \frac{1}{945}$$



The Sylvester's determinant  $D(f_1, f_2)$  is equal to  
80384/41351522625  $\square$

Case 1.1.  $\rho_1 = \rho_2$ .

From (E-45) and (E-57), the assumption gives  $\rho_1 = \rho_2 = \frac{1}{7}$ .  
Due to Lemma 1.7.1, we lead to a contradiction.

Case 1.2.  $\rho_1 = \rho_3$

We may assume that  $\rho_1, \rho_2, \rho_4$  are distinct. From  
(E-0), (E-1) and (E-21), we have the equation

$$(1.7.9) \quad \begin{pmatrix} 1 & 1 & 1 \\ \rho_1 & \rho_2 & \rho_4 \\ \rho_1^2 & \rho_2^2 & \rho_4^2 \end{pmatrix} \begin{pmatrix} v_1+v_3 \\ v_2 \\ v_4 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{6} \\ \frac{1}{12} \end{pmatrix}$$

The solution of (9) is given by

$$\begin{pmatrix} v_1+v_3 \\ v_2 \\ v_4 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ \rho_1 & \rho_2 & \rho_4 \\ \rho_1^2 & \rho_2^2 & \rho_4^2 \end{pmatrix}^{-1} \begin{pmatrix} \frac{1}{2} \\ \frac{1}{6} \\ \frac{1}{12} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{-6\rho_2\rho_4+2(\rho_2+\rho_4)-1}{12(\rho_1-\rho_2)(\rho_4-\rho_1)} \\ \frac{-6\rho_4\rho_1+2(\rho_4+\rho_1)-1}{12(\rho_1-\rho_2)(\rho_2-\rho_4)} \\ \frac{-6\rho_1\rho_2+2(\rho_1+\rho_2)-1}{12(\rho_2-\rho_4)(\rho_4-\rho_1)} \end{pmatrix}$$

Note that  $v_1+v_3$ ,  $v_2$ ,  $v_4$  can not vanish. The reason is as follows: For example, assume that  $-6\rho_2\rho_4+2(\rho_2+\rho_4)-1 = 0$ . Then,

$$\rho_4 = \frac{2\rho_2 - 1}{6\rho_2 - 2}$$

Holds Substituting this into the cubic equation

$$\rho_4^3 - \frac{9}{7}\rho_4^2 + \frac{3}{7}\rho_4 - \frac{1}{35} = 0,$$

we see that

$$\frac{64\rho_2^3 - 24\rho_2^2 - 12\rho_2 + 3}{35(6\rho_2-2)^3} = 0$$

But, by Lemma 1.7.2, there is no common roots for the cubic equations

$$\rho_2^3 - \frac{9}{7}\rho_2^2 + \frac{3}{7}\rho_2 - \frac{1}{35} = 0$$

and

$$\rho_2^3 - \frac{3}{8}\rho_2^2 - \frac{3}{16}\rho_2 + \frac{3}{64} = 0$$

Then, from the equations (1) and (2) we have

$$v_1 A_1 + v_3 A_3 = v_2 A_2 = v_4 A_4 = 0$$

and

$$v_1 B_1 + v_3 B_3 = v_2 B_2 = v_4 B_4 = 0.$$

Since  $v_2 \neq 0$ ,  $A_2=B_2=0$  holds. This means the equations  $\tau_{21} = \frac{1}{2}\rho_2^2$  and  $\rho_1 \tau_{21} = \frac{1}{6}\rho_2^3$ , which imply  $3\rho_1 = \rho_2$ . Hence, we lead to a contradiction by virtue of Lemma 1.7. 3

Case 1.3.  $\rho_1 = \rho_4$

This is equivalent to Case 1.2

Case 1.4  $\rho_2 = \rho_3$

We can assume that  $\rho_1, \rho_2, \rho_4$  are distinct. From (E-0), (E-1), (E-21), we have the solution

$$\begin{aligned} v_1 &= \frac{-6\rho_2\rho_4 + 2(\rho_2+\rho_4)-1}{12(\rho_1-\rho_2)(\rho_4-\rho_1)} \\ v_2+v_3 &= \frac{-6\rho_4\rho_1 + 2(\rho_4+\rho_1)-1}{12(\rho_1-\rho_2)(\rho_2-\rho_4)}, \\ v_4 &= \frac{-6\rho_1\rho_2 + 2(\rho_1+\rho_2)-1}{12(\rho_2-\rho_4)(\rho_4-\rho_1)} \end{aligned}$$

Note that each numerator on the right can not vanish by the same reason as in Case 1.2. Then, (1) implies  $v_1 A_1 = v_2 A_2 + v_3 A_3 = v_4 A_4 = 0$ . Since  $v_1 \neq 0$ , we see  $A_1 = 0$ , which means  $\rho_1 = 0$ . Thus, we lead to a contradiction.

Case 1.5.  $\rho_2 = \rho_4$

and

Case 1.6.  $\rho_3 = \rho_4$

Both of them are equivalent to Case 1.4.

Case 2. No two of  $\rho_1, \rho_2, \rho_3, \rho_4$  are equal.

The equation (1) implies  $v_1 A_1 = v_2 A_2 = v_3 A_3 = v_4 A_4 = 0$

Thus, we distinguish cases according as  $v_i$  or  $A_i$  vanishes.

We have, however, the following results.

Lemma 1.7.4 The case of  $v_J = v_K - v_L = 0$  can not occur

Proof In this case,  $v_I = \frac{1}{2}$  by (E-0). Then, (E-1) implies  $\rho_I = \frac{1}{3}$  But, they do not satisfy (E-21).  $\square$

Lemma 1.7.5 The case for  $v_K = v_L = 0$  leads to a contradiction.

Proof The equation  $v_K - v_L = 0$  yields a linear system

$$v_I + v_J = \frac{1}{2},$$

$$\rho_I v_I + \rho_J v_J = \frac{1}{6}$$

by (E-0), (E-1) Since  $\rho_I \neq \rho_J$ , this system has the solution

$$v_I = \frac{1 - 3\rho_J}{6(\rho_I - \rho_J)}, \quad v_J = \frac{1 - 3\rho_I}{6(\rho_J - \rho_I)}$$

Substitution of this into (E-21) and (E-31) implies

$$\frac{1}{6}(\rho_I + \rho_J) - \frac{1}{2}\rho_I\rho_J = \frac{1}{12},$$

$$\frac{1}{6}(\rho_I^2 + \rho_I\rho_J + \rho_J^2) - \frac{1}{2}\rho_I\rho_J(\rho_I + \rho_J) = \frac{1}{20}.$$

Put  $X = \rho_I + \rho_J$ ,  $Y = \rho_I\rho_J$ , we have

$$2X - 6Y = 1,$$

$$10(X^2 - Y) - 30XY = 3.$$

Thus, we easily see that  $X = \frac{4}{5}$ ,  $Y = \frac{1}{10}$ . That is,  $\rho_I$  and  $\rho_J$  are equal to the roots of the quadratic equation

$$(1.7.10) \quad x^2 - \frac{4}{5}x + \frac{1}{10} = 0,$$

which has real distinct roots. On the other hand, we see that

$$\begin{aligned} \text{the left on (E-41)} &= v_I\rho_I^4 + v_J\rho_J^4 \\ &= \frac{1}{6}(\rho_I + \rho_J)(\rho_I^2 + \rho_J^2) - \frac{1}{2}\rho_I\rho_J(\rho_I^2 + \rho_I\rho_J + \rho_J^2) \\ &= \frac{19}{600} \end{aligned}$$

which is a contradiction.  $\square$

Due to the above Lemmas, we distinguish five cases.

Case 2.1.  $v_1 = 0$  and  $A_2 = A_3 = A_4 = 0$  By a similar consideration as in Case 1, we see that  $\rho_2, \rho_3, \rho_4$  satisfy

$$\rho_2 + \rho_3 + \rho_4 = \frac{9}{7},$$

$$\rho_2\rho_3 + \rho_3\rho_4 + \rho_4\rho_2 = \frac{3}{7},$$

$$\rho_2\rho_3\rho_4 = \frac{1}{35}$$

Hence, they are equal to the distinct roots of the cubic equation (3). Note that, contrary to Case 1,  $\rho_1$  is equal to none of them.

On the other hand, the equation (2) yields  $v_2B_2 = v_3B_3 = v_4B_4 = 0$ . Taking Lemma 1.7.5 into account, we are sufficient to consider the case  $B_2 = B_3 = B_4 = 0$ .

$A_2 = B_2 = 0$  implies the equations  $\tau_{21} = \frac{1}{2}\rho_2^2$  and  $\rho_1\tau_{21} = \frac{1}{6}\rho_2^3$ , which give  $\rho_1 = \frac{1}{3}\rho_2$ .  $A_3 = B_3 = 0$  implies a linear system

$$\tau_{31} + \tau_{32} = \frac{1}{2}\rho_3^2,$$

$$\rho_1\tau_{31} + \rho_2\tau_{32} = \frac{1}{6}\rho_3^3,$$

which has the solution

$$(1.7.11) \quad \tau_{31} = \frac{\rho_3^2(3\rho_2 - \rho_3)}{4\rho_2}, \quad \tau_{32} = \frac{\rho_3^2(\rho_3 - \rho_2)}{4\rho_2}.$$

Since  $\rho_2, \rho_3, \rho_4$  are distinct, (E-0), (E-1), (E-21) give

the solution for  $v_2, v_3, v_4$  as

$$(1.7 \ 12) \quad \begin{cases} v_2 = \frac{-6\rho_3\rho_4+2(\rho_3+\rho_4)-1}{12(\rho_2-\rho_3)(\rho_4-\rho_2)}, \\ v_3 = \frac{-6\rho_4\rho_2+2(\rho_4+\rho_2)-1}{12(\rho_2-\rho_3)(\rho_3-\rho_4)}, \\ v_4 = \frac{-6\rho_2\rho_3+2(\rho_2+\rho_3)-1}{12(\rho_3-\rho_4)(\rho_4-\rho_2)} \end{cases}$$

(E-44) gives the equation

$$\begin{aligned} v_4(\rho_1^2\tau_{41}+\rho_2^2\tau_{42}+\rho_3^2\tau_{43}) &= \frac{1}{360}-v_2\rho_1^2\tau_{21}-v_3(\rho_1^2\tau_{31}+\rho_2^2\tau_{32}) \\ &= \frac{1}{360}-\frac{1}{18}v_2\rho_2^4-v_3\rho_2^2(\frac{1}{9}\tau_{31}+\tau_{32}) \\ &= \frac{1}{360}-\frac{1}{18}v_2\rho_2^4-\frac{1}{18}v_3\rho_2^2(4\rho_3-3\rho_2) \end{aligned}$$

by (9) Hence, we may represent the left on (E-54) as the polynomial of  $\rho_2$  and  $\rho_3$  By (9) and (10),

$$\begin{aligned} &v_2\rho_2\rho_1^2\tau_{21}+v_3\rho_3(\rho_1^2\tau_{31}+\rho_2^2\tau_{32})+v_4\rho_4(\rho_1^2\tau_{41}+\rho_2^2\tau_{42}+\rho_3^2\tau_{43})-\frac{1}{504} \\ &= \frac{1}{18}v_2\rho_2^5+\frac{1}{18}v_3\rho_2\rho_3^3(4\rho_3-3\rho_2)+\frac{\rho_4}{360}-\frac{1}{18}v_2\rho_2^4\rho_4-\frac{1}{18}v_3\rho_2\rho_3^2\rho_4(4\rho_3-3\rho_2)-\frac{1}{504} \\ &= \frac{1}{37800(\rho_2-\rho_3)}(525\rho_2^2\rho_3^2-360\rho_2^2\rho_3-420\rho_2\rho_3^2-5\rho_2^2+260\rho_2\rho_3+105\rho_3^2-60\rho_3+3) \end{aligned}$$

Let us denote the numerator of the above by  $\varphi(\rho_2, \rho_3)$

The question is whether  $\varphi(\rho_2, \rho_3)$  vanishes for any pair  $(\rho_2, \rho_3)$ . We have known the values  $R_0, R_1, R_{-1}$  which  $\rho_2$  and  $\rho_3$  are possible to be equal to. Calculation shows the following:

$$\begin{aligned}\varphi(R_0, R_1) = \frac{4}{343} & (-420\cos^2\theta - 760\sqrt{3}\sin\theta \cdot \cos\theta - 630\sqrt{2}\cos\theta + 60\sqrt{6}\sin\theta \\ & + 189 + 42\sqrt{3}),\end{aligned}$$

$$\begin{aligned}\varphi(R_0, R_{-1}) = \frac{4}{343} & (-420\cos^2\theta + 760\sqrt{3}\sin\theta \cdot \cos\theta - 630\sqrt{2}\cos\theta - 60\sqrt{6}\sin\theta \\ & + 189 - 42\sqrt{3}),\end{aligned}$$

$$\begin{aligned}\varphi(R_1, R_0) = \frac{4}{343} & (1350\cos^2\theta - 170\sqrt{3}\cos\theta \cdot \sin\theta + 405\sqrt{2}\cos\theta - 285\sqrt{6}\sin\theta \\ & - 696 - 42\sqrt{3}),\end{aligned}$$

$$\begin{aligned}\varphi(R_1, R_{-1}) = \frac{4}{343} & (-930\cos^2\theta + 590\sqrt{3}\sin\theta \cdot \cos\theta + 225\sqrt{2}\cos\theta - 345\sqrt{6}\sin\theta \\ & + 444 + 42\sqrt{3}),\end{aligned}$$

$$\begin{aligned}\varphi(R_{-1}, R_0) = \frac{4}{343} & (1350\cos^2\theta + 170\sqrt{3}\sin\theta \cos\theta + 405\sqrt{2}\cos\theta + 285\sqrt{6}\sin\theta \\ & - 696 + 42\sqrt{3}),\end{aligned}$$

$$\begin{aligned}\varphi(R_{-1}, R_1) = \frac{4}{343} & (-930\cos^2\theta - 590\sqrt{3}\sin\theta \cdot \cos\theta + 225\sqrt{2}\cos\theta + 345\sqrt{6}\sin\theta \\ & + 444 - 42\sqrt{3})\end{aligned}$$

Computation by interval arithmetic shows the following:



$$\varphi(R_0, R_1) \in [-11.6391, -11.6390],$$

$$\varphi(R_0, R_{-1}) \in [-4.70784, -4.70783],$$

$$\varphi(R_1, R_0) \in [3.20479, 3.20480],$$

$$\varphi(R_1, R_{-1}) \in [0.821791, 0.821792],$$

$$\varphi(R_{-1}, R_0) \in [12.1750, 12.1751],$$

$$\varphi(R_{-1}, R_1) \in [-0.956777, -0.956776]$$

(On the interval arithmetic, see [8] Above calculation is carried out by the program made by K. Ichida on HITAC VOS3 at the Educational Center for Information Processing, Kyoto Univ ) None of them vanishes under the condition (4) because every interval given above is away from zero Thus, we have a contradiction.

Case 2.2.  $v_2 = 0$  and  $A_1 = A_3 = A_4 = 0$   $A_1 = 0$  implies  $\rho_1 = 0$  Then,  $\rho_2, \rho_3, \rho_4$  can not vanish. From (E-1), (E-21), we have

$$v_3 = \frac{1-2\rho_4}{12\rho_3(\rho_3-\rho_4)}, \quad v_4 = \frac{1-2\rho_3}{12\rho_4(\rho_4-\rho_3)}.$$

Substituting these into (E-31), (E-41), we see that

$$\rho_3 + \rho_4 - 2\rho_3\rho_4 = \frac{3}{5},$$

$$(\rho_3 + \rho_4)^2 - 2\rho_3\rho_4(\rho_3 + \rho_4) - \rho_3\rho_4 = \frac{2}{5}.$$

Put  $X = \rho_3 + \rho_4$ ,  $Y = \rho_3 \rho_4$ , then we have  $X = 1$ ,  $Y = \frac{1}{5}$ . The left on (E-51) is equal to

$$\begin{aligned} & \frac{1}{12}(-2\rho_3^3\rho_4 - 2\rho_3\rho_4^3 - 2\rho_3^2\rho_4^2 + \rho_3^3 + \rho_3^2\rho_4 + \rho_3\rho_4^2 + \rho_4^3) \\ &= \frac{1}{12}(X^3 - 2(X^2 - Y)Y - 2(X + Y)Y) = \frac{1}{100}, \end{aligned}$$

which is a contradiction.

Case 2.3  $v_3 = 0$  and  $A_1 = A_2 = A_4 = 0$ . Equivalent to Case 2.2

Case 2.4  $v_4 = 0$  and  $A_1 = A_2 = A_3 = 0$  Equivalent to Case 2.2.

Case 2.5.  $A_1 = A_2 = A_3 = A_4 = 0$ .  $A_1 = 0$  implies  $\rho_1 = 0$ , which means  $B_1 = 0$ . Then, the equations  $\{v_i B_i = \{v_i \rho_i B_i = \{v_i \rho_i^2 B_i = 0$  yield  $v_2 B_2 = v_3 B_3 = v_4 B_4 = 0$ . Since  $v_2, v_3, v_4$  are assumed to be non-zero, we have  $B_2 = B_3 = B_4 = 0$ .  $B_2 = \rho_1 \tau_{21} - \frac{1}{6} \rho_2^3 = 0$  implies  $\rho_2 = 0$  because  $\rho_1 = 0$ . This contradicts the assumption that no two of  $\rho_i$  are equal.

Now, we have accomplished to investigate the whole cases. In conclusion, we have

Theorem 8 The explicit (1,4)-stage formula can not attain order 7 Its attainable order is 6.

Note. Shintani gives (1,4)-stage formula with parameters  
 $v_1 = \frac{1}{20}$ ,  $v_2 = 7(7+\sqrt{21})/360$ ,  $v_3 = 8/45$ ,  $v_4 = 7(7-\sqrt{21})/360$ ,  
 $\rho_1 = 0$ ,  $\rho_2 = (7-\sqrt{21})/14$ ,  $\tau_{21} = (5-\sqrt{21})/28$ ,  $\rho_3 = \frac{1}{2}$ ,  $\tau_{31} =$   
 $(3-\sqrt{21})/192$ ,  $\tau_{32} = (21+\sqrt{21})/192$ ,  $\rho_4 = (7+\sqrt{21})/14$ ,  $\tau_{41} =$   
 $(21+5\sqrt{21})/294$ ,  $\tau_{42} = (\sqrt{21}-3)/84$ ,  $\tau_{43} = (21+\sqrt{21})/147$  These  
parameters are also not unique solution of (E-0)  $\sim$  (E-46).

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Table 1.

$$\kappa_0 = g_0$$

$$\kappa_1 = [D_0 g]_0$$

$$\kappa_2 = [D_0^2 g]_0 + g_0 g_{y,0}$$

$$\kappa_3 = [D_0^3 g]_0 + [D_0 g]_0 g_{y,0} + 3g_0 [D_0 g_y]_0$$

$$\begin{aligned} \kappa_4 = & [D_0^4 g]_0 + [D_0^2 g]_0 g_{y,0} + 4[D_0 g]_0 [D_0 g_y]_0 + 6g_0 [D_0^2 g_y]_0 + g_0 g_{y,0}^2 \\ & + 3g_0^2 g_{yy,0} \end{aligned}$$

$$\begin{aligned} \kappa_5 = & [D_0^5 g]_0 + [D_0^3 g]_0 g_{y,0} + 5[D_0^2 g]_0 [D_0 g_y]_0 + 10[D_0 g]_0 [D_0^2 g_y]_0 \\ & + 10g_0 [D_0^3 g_y]_0 + [D_0 g]_0 g_{y,0}^2 + 8g_0 g_{y,0} [D_0 g_y]_0 + 10g_0 [D_0 g]_0 g_{yy,0} \\ & + 15g_0^2 [D_0 g_{yy}]_0 \end{aligned}$$

$$\begin{aligned} \kappa_6 = & [D_0^6 g]_0 + [D_0^4 g]_0 g_{y,0} + 6[D_0^3 g]_0 [D_0 g_y]_0 + 15[D_0^2 g]_0 [D_0^2 g_y]_0 \\ & + 20[D_0 g]_0 [D_0^3 g_y]_0 + 15g_0 [D_0^4 g_y]_0 + [D_0^2 g]_0 g_{y,0}^2 + 18g_0 [D_0 g_y]_0^2 \\ & + 10[D_0 g]_0 g_{y,0} [D_0 g_y]_0 + 21g_0 g_{y,0} [D_0^2 g_y]_0 + 10[D_0 g]_0^2 g_{yy,0} \\ & + 15g_0 [D_0^2 g]_0 g_{yy,0} + 60g_0 [D_0 g]_0 [D_0 g_{yy}]_0 + 45g_0^2 [D_0^2 g_{yy}]_0 \end{aligned}$$

$$+ g_0 \cdot g_{y,0}^3 + 18g_0^2 \cdot g_{y,0} \cdot g_{yy,0} + 15g_0^3 \cdot g_{yyy,0}$$

$$\begin{aligned} \kappa_7 = & [D_0^7 g]_0 + [D_0^5 g]_0 \cdot g_{y,0} + 7[D_0^4 g]_0 [D_0 g_y]_0 + 21[D_0^3 g]_0 [D_0^2 g_y]_0 \\ & + [D_0^3 g]_0 \cdot g_{y,0}^2 + 35[D_0^2 g]_0 [D_0^3 g_y]_0 + 12[D_0^2 g]_0 g_{y,0} [D_0 g_y]_0 \\ & + 35[D_0 g]_0 [D_0^4 g_y]_0 + 28[D_0 g]_0 [D_0 g_y]_0^2 + 31[D_0 g]_0 \cdot g_{y,0} [D_0^2 g_y]_0 \\ & + [D_0 g]_0 \cdot g_{y,0}^3 + 35[D_0 g]_0 [D_0^2 g]_0 \cdot g_{yy,0} + 70[D_0 g]_0^2 [D_0 g_{yy}]_0 \\ & + 21g_0 [D_0^5 g_y]_0 + 105g_0 [D_0 g_y]_0 [D_0^2 g_y]_0 + 45g_0 \cdot g_{y,0} [D_0^3 g_y]_0 \\ & + 15g_0 g_{y,0}^2 [D_0 g_y]_0 + 21g_0 [D_0^3 g]_0 g_{yy,0} + 105g_0 [D_0^2 g]_0 [D_0 g_{yy}]_0 \\ & + 210g_0 [D_0 g]_0 [D_0^2 g_{yy}]_0 + 66g_0 [D_0 g]_0 g_{y,0} g_{yy,0} + 105g_0^2 \cdot [D_0^3 g_{yy}]_0 \\ & + 84g_0^2 [D_0 g_y]_0 \cdot g_{yy,0} + 120g_0^2 g_{y,0} [D_0 g_{yy}]_0 + 105g_0^2 [D_0 g]_0 \cdot g_{yyy,0} \\ & + 105g_0^3 \cdot [D_0 g_{yyy}]_0 \end{aligned}$$

$$\begin{aligned} \kappa_8 = & [D_0^8 g]_0 + [D_0^6 g]_0 \cdot g_{y,0} + 8[D_0^5 g]_0 [D_0 g_y]_0 + 28[D_0^4 g]_0 [D_0^2 g_y]_0 \\ & + [D_0^4 g]_0 \cdot g_{y,0}^2 + 56[D_0^3 g]_0 [D_0^3 g_y]_0 + 14[D_0^3 g]_0 g_{y,0} [D_0 g_y]_0 \\ & + 70[D_0^2 g]_0 [D_0^4 g_y]_0 + 40[D_0^2 g]_0 \cdot [D_0 g_y]_0^2 + 43[D_0^2 g]_0 g_{y,0} [D_0^2 g_y]_0 \\ & + [D_0^2 g]_0 g_{y,0}^3 + 35[D_0^2 g]_0^2 \cdot g_{yy,0} + 56[D_0 g]_0 [D_0^5 g_y]_0 \end{aligned}$$

$$\begin{aligned}
& + 192[D_0 g]_0 [D_0 g_y]_0 [D_0^2 g_y]_0 + 76[D_0 g]_0 g_{y,0} \cdot [D_0^3 g_y]_0 \\
& + 18[D_0 g]_0 \cdot g_{y,0}^2 \cdot [D_0 g_y]_0 + 56[D_0 g]_0 [D_0^3 g]_0 \cdot g_{yy,0} \\
& + 280[D_0 g]_0 [D_0^2 g]_0 [D_0 g_{yy}]_0 + 280[D_0 g]_0^2 \cdot [D_0^2 g_{yy}]_0 \\
& + 66[D_0 g]_0^2 \cdot g_{y,0} g_{yy,0} + 28g_0 [D_0^6 g_y]_0 + 168g_0 \cdot [D_0^2 g_y]_0^2 \\
& + 248g_0 [D_0 g_y]_0 \cdot [D_0^3 g_y]_0 + 85g_0 g_{y,0} [D_0^4 g_y]_0 + 82g_0 g_{y,0} \cdot [D_0 g_y]_0^2 \\
& + 49g_0 g_{y,0}^2 [D_0^2 g_y]_0 + g_0 g_{y,0}^4 + 28g_0 [D_0^4 g]_0 g_{yy,0} \\
& + 168g_0 [D_0^3 g]_0 [D_0 g_{yy}]_0 + 420g_0 [D_0^2 g]_0 [D_0^2 g_{yy}]_0 \\
& + 113g_0 [D_0^2 g]_0 g_{y,0} g_{yy,0} + 560g_0 [D_0 g]_0 [D_0^3 g_{yy}]_0 \\
& + 360g_0 [D_0 g]_0 [D_0 g_y]_0 g_{yy,0} + 508g_0 [D_0 g]_0 g_{y,0} [D_0 g_{yy}]_0 \\
& + 280g_0 [D_0 g]_0^2 g_{yyy,0} + 210g_0^2 \cdot [D_0^4 g_{yy}]_0 \\
& + 252g_0^2 [D_0^2 g_y]_0 \cdot g_{yy,0} + 624g_0^2 \cdot [D_0 g_y]_0 \cdot [D_0 g_{yy}]_0 \\
& + 465g_0^2 \cdot g_{y,0} [D_0^2 g_{yy}]_0 + 81g_0^2 g_{y,0}^2 g_{yy,0} + 210g_0^2 [D_0^2 g]_0 \cdot g_{yyy,0} \\
& + 840g_0^2 [D_0 g]_0 [D_0 g_{yyy}]_0 + 420g_0^3 [D_0^2 g_{yy}]_0 + 84g_0^3 \cdot g_{yy,0}^2 \\
& + 225g_0^3 \cdot g_{y,0} g_{yyy,0} + 105g_0^4 g_{yyyy,0}
\end{aligned}$$



Table 2.

$$\kappa_{10} = g_0$$

$$\kappa_{11} = \rho_1 [D_0 g]_0$$

$$\kappa_{12} = \rho_1^2 [D_0^2 g]_0 + 2 T_{10} \cdot g_0 g_{y,0}$$

$$\kappa_{13} = \rho_1^3 [D_0^3 g]_0 + 6 T_{11} [D_0 g]_0 \cdot g_{y,0} + 6 \rho_1 T_{10} \cdot g_0 [D_0 g_y]_0$$

$$\begin{aligned} \kappa_{14} = & \rho_1^4 [D_0^4 g]_0 + 12 T_{12} [D_0^2 g]_0 g_{y,0} + 24 \rho_1 T_{11} [D_0 g]_0 [D_0 g_y]_0 \\ & + 12 \rho_1^2 T_{10} g_0 [D_0^2 g_y]_0 + 24 \left( \sum_j \tau_{1j} T_{j0} \right) g_0 g_{y,0}^2 + 12 T_{10}^2 g_0^2 \cdot g_{y,0} \end{aligned}$$

$$\begin{aligned} \kappa_{15} = & \rho_1^5 [D_0^5 g]_0 + 20 T_{13} \cdot [D_0^3 g]_0 g_{y,0} + 60 \rho_1 T_{12} [D_0^2 g]_0 [D_0 g_y]_0 \\ & + 60 \rho_1^2 T_{11} [D_0 g]_0 [D_0^2 g_y]_0 + 120 \left( \sum_j \tau_{1j} T_{j1} \right) [D_0 g]_0 g_{y,0}^2 \\ & + 20 \rho_1^3 T_{10} \cdot g_0 \cdot [D_0^3 g_y]_0 + 120 \left\{ \sum_j (\rho_1 + \rho_j) \tau_{1j} T_{j0} \right\} g_0 \cdot g_{y,0} [D_0 g_y]_0 \\ & + 120 T_{10} T_{11} g_0 [D_0 g]_0 g_{yy,0} + 60 \rho_1 T_{10}^2 \cdot g_0^2 \cdot [D_0 g_{yy}]_0 \end{aligned}$$

$$\begin{aligned} \kappa_{16} = & \rho_1^6 [D_0^6 g]_0 + 30 T_{14} [D_0^4 g]_0 g_{y,0} + 120 \rho_1 T_{13} [D_0^3 g] \cdot [D_0 g_y]_0 \\ & + 180 \rho_1^2 T_{12} [D_0^2 g]_0 [D_0^2 g_y]_0 + 360 \left( \sum_j \tau_{1j} T_{j2} \right) [D_0^2 g]_0 g_{y,0}^2 \\ & + 120 \rho_1^3 T_{11} [D_0 g]_0 [D_0^3 g_y]_0 + 720 \left\{ \sum_j (\rho_1 + \rho_j) \tau_{1j} T_{j1} \right\} [D_0 g]_0 g_{y,0} [D_0 g_y]_0 \end{aligned}$$

$$\begin{aligned}
& + 360T_{11}^2 [D_0 g]_0^2 \cdot g_{yy,0} + 30\rho_1^4 T_{10} g_0 [D_0^4 g_y]_0 \\
& + 720(\sum_j \rho_1 \rho_j \tau_{1j} T_{j0}) g_0 [D_0 g_y]_0^2 + 360(\sum_j (\rho_1^2 + \rho_j^2) \tau_{1j} T_{j0}) g_0 \cdot g_{y,0} \cdot [D_0^2 g_y]_0 \\
& + 720(\sum_{jk} \tau_{1j} \tau_{jk} T_{k0}) g_0 \cdot g_{y,0}^3 + 360T_{10} T_{12} g_0 [D_0^2 g]_0 \cdot g_{yy,0} \\
& + 720\rho_1 T_{10} T_{11} g_0 [D_0 g]_0 [D_0 g_{yy}]_0 + 180\rho_1^2 T_{10}^2 g_0^2 [D_0^2 g_{yy}]_0 \\
& + 360(\sum_j \tau_{1j} (T_{j0}^2 + 2T_{10} T_{j0})) g_0^2 \cdot g_{y,0} g_{yy,0} + 120T_{10}^3 \cdot g_0^3 \cdot g_{yyy,0} \\
\kappa_{17} = & \rho_1^7 [D_0^7 g]_0 + 42T_{15} [D_0^5 g]_0 g_{y,0} + 210\rho_1 T_{14} [D_0^4 g]_0 \cdot [D_0 g_y]_0 \\
& + 420\rho_1^2 T_{13} [D_0^3 g]_0 [D_0^2 g_y]_0 + 840(\sum_j \tau_{1j} T_{j3}) [D_0^3 g]_0 \cdot g_{y,0}^2 \\
& + 420\rho_1^3 T_{12} [D_0^2 g]_0 \cdot [D_0^3 g_y]_0 + 2520(\sum_j (\rho_1 + \rho_j) \tau_{1j} T_{j2}) [D_0^2 g]_0 \cdot g_{y,0} \cdot [D_0 g_y]_0 \\
& + 210\rho_1^4 T_{11} [D_0 g]_0 [D_0^4 g_y]_0 + 5040(\sum_j \rho_1 \rho_j \tau_{1j} T_{j1}) [D_0 g]_0 [D_0 g_y]_0^2 \\
& + 2520(\sum_j (\rho_1^2 + \rho_j^2) \tau_{1j} T_{j1}) [D_0 g]_0 g_{y,0} [D_0^2 g_y]_0 \\
& + 5040(\sum_{jk} \tau_{1j} \tau_{jk} T_{k1}) [D_0 g]_0 \cdot g_{y,0}^3 + 2520T_{11} T_{12} [D_0 g]_0 [D_0^2 g]_0 \cdot g_{yy,0} \\
& + 2520\rho_1 T_{11}^2 [D_0 g]_0^2 [D_0 g_{yy}]_0 + 42\rho_1^5 T_{10} g_0 [D_0^5 g_y]_0 \\
& + 2520(\sum_j \rho_1 \rho_j (\rho_1 + \rho_j) \tau_{1j} T_{j0}) g_0 [D_0 g_y]_0 [D_0^2 g_y]_0 \\
& + 840(\sum_j (\rho_1^3 + \rho_j^3) \tau_{1j} T_{j0}) g_0 \cdot g_{y,0} [D_0^3 g_y]_0
\end{aligned}$$

$$\begin{aligned}
& + 5040 \left( \sum_{j,k} (\rho_i + \rho_j + \rho_k) \tau_{ij} \tau_{jk} T_{k0} \right) g_0 \cdot g_{y,0}^2 [D_0 g_y]_0 \\
& + 840 T_{10} T_{13} g_0 [D_0^3 g]_0 \cdot g_{yy,0} + 2520 \rho_1 T_{10} T_{12} g_0 [D_0^2 g]_0 \cdot [D_0 g_{yy}]_0 \\
& + 2520 \rho_1^2 T_{10} T_{11} g_0 [D_0 g]_0 [D_0^2 g_{yy}]_0 + 5040 \left( \sum_j \tau_{ij} (T_{10} T_{j1} + T_{j0} T_{j1} + T_{j0} T_{11}) \right) g_0 \cdot \\
& [D_0 g]_0 g_{y,0} g_{yy,0} + 420 \rho_1^3 T_{10}^2 g_0^2 \cdot [D_0^3 g_{yy}]_0 \\
& + 2520 \left( \sum_j (2 \rho_1 T_{10} + \rho_j T_{j0}) \tau_{ij} T_{j0} \right) g_0^2 \cdot [D_0 g_y]_0 \cdot g_{yy,0} \\
& + 2520 \left( \sum_j (\rho_1 T_{j0} + 2 \rho_j T_{10}) \tau_{ij} T_{j0} \right) g_0^2 \cdot g_{y,0} \cdot [D_0 g_{yy}]_0 \\
& + 2520 T_{10}^2 T_{11} g_0^2 [D_0 g]_0 \cdot g_{yyy,0} + 840 \rho_1 T_{10}^3 g_0^3 \cdot [D_0 g_{yyy}]_0 \\
\kappa_{18} = & \rho_1^8 [D_0^8 g]_0 + 56 T_{16} \cdot [D_0^6 g]_0 \cdot g_{y,0} + 336 \rho_1 T_{15} [D_0^5 g]_0 [D_0 g_y]_0 \\
& + 840 \rho_1^2 T_{14} [D_0^4 g]_0 [D_0^2 g_y]_0 + 1680 \left( \sum_j \tau_{ij} T_{j4} \right) [D_0^4 g]_0 \cdot g_{y,0}^2 \\
& + 1120 \rho_1^3 T_{13} [D_0^3 g]_0 [D_0^3 g_y]_0 + 6720 \left( \sum_j (\rho_1 + \rho_j) \tau_{ij} T_{j3} \right) [D_0^3 g]_0 \cdot g_{y,0} \cdot [D_0 g_y]_0 \\
& + 840 \rho_1^4 T_{12} [D_0^2 g]_0 [D_0^4 g_y]_0 + 20160 \left( \sum_j \rho_1 \rho_j \tau_{ij} T_{j2} \right) [D_0^2 g]_0 [D_0 g_y]_0^2 \\
& + 10080 \left( \sum_j (\rho_1^2 + \rho_j^2) \tau_{ij} T_{j2} \right) [D_0^2 g]_0 \cdot g_{y,0} [D_0^2 g_y]_0 \\
& + 20160 \left( \sum_{j,k} \tau_{ij} \tau_{jk} T_{k2} \right) [D_0^2 g]_0 g_{y,0}^3 + 5040 T_{12}^2 [D_0^2 g]_0^2 \cdot g_{yy,0} \\
& + 336 \rho_1^5 T_{11} [D_0 g]_0 [D_0^5 g_y]_0 + 20160 \left( \sum_j \rho_1 \rho_j (\rho_1 + \rho_j) \tau_{ij} T_{j1} \right) [D_0 g]_0 \cdot [D_0 g_y]_0 \cdot [D_0^2 g_y]_0
\end{aligned}$$

$$\begin{aligned}
& + 6720(\sum_j(\rho_i^3 + \rho_j^3)\tau_{ij}T_{j1})[D_0g]_0 \cdot g_{y,0} \cdot [D_0^3g_y]_0 \\
& + 40320(\sum_{jk}(\rho_i + \rho_j + \rho_k)\tau_{ij}\tau_{jk}T_{k1})[D_0g]_0 \cdot g_{y,0}^2 [D_0g_y]_0 \\
& + 6720T_{11}T_{13}[D_0g]_0 [D_0^3g]_0 g_{yy,0} + 20160\rho_iT_{11}T_{12}[D_0g]_0 \\
& [D_0^2g]_0 [D_0g_{yy}]_0 + 10080\rho_i^2T_{11}^2[D_0g]_0^2 [D_0^2g_{yy}]_0 \\
& + 20160(\sum_j\tau_{ij} T_{j1}(2T_{11}+T_{j1}))[D_0g]_0^2 \cdot g_{y,0} g_{yy,0} \\
& + 56\rho_i^6T_{10}g_0 [D_0^6g_y]_0 + 10080(\sum_j\rho_i^2\rho_j^2\tau_{ij}T_{j0})g_0 \cdot [D_0^2g_y]_0^2 \\
& + 6720(\sum_j\rho_i\rho_j(\rho_i^2 + \rho_j^2)\tau_{ij}T_{j0})g_0 [D_0g_y]_0 [D_0^3g_y]_0 \\
& + 1680(\sum_j(\rho_i^4 + \rho_j^4)\tau_{ij}T_{j0})g_0 g_{y,0} [D_0^4g_y]_0 \\
& + 40320(\sum_{jk}(\rho_i\rho_j + \rho_j\rho_k + \rho_i\rho_k)\tau_{ij}\tau_{jk}T_{k0})g_0 g_{y,0} [D_0g_y]_0^2 \\
& + 20160(\sum_{jk}(\rho_i^2 + \rho_j^2 + \rho_k^2)\tau_{ij}\tau_{jk}T_{k0})g_0 g_{y,0}^2 [D_0^2g_y]_0 \\
& + 40320(\sum_{jkl}\tau_{ij}\tau_{jk}\tau_{kl}T_{l0})g_0 g_{y,0}^4 + 1680T_{10}T_{14}g_0 [D_0^4g]_0 \cdot g_{yy,0} \\
& + 6720\rho_iT_{10}T_{13}g_0 [D_0^3g]_0 [D_0g_{yy}]_0 \\
& + 10080\rho_i^2T_{10}T_{12}g_0 \cdot [D_0^2g]_0 [D_0^2g_{yy}]_0 \\
& + 20160(\sum_j\tau_{ij}(T_{12}T_{j0} + T_{10}T_{j2} + T_{j0}T_{j2}))g_0 [D_0^2g]_0 g_{y,0} g_{yy,0}
\end{aligned}$$

$$\begin{aligned}
& + 6720\rho_1^3 T_{10} T_{11} \varepsilon_0 \cdot [D_0 \varepsilon]_0 \cdot [D_0^3 \varepsilon_{yy}]_0 \\
& + 40320 \left( \sum_j \tau_{1j} (\rho_j T_{10} T_{j1} + \rho_j T_{11} T_{j0} + \rho_1 T_{j0} T_{j1}) \right) \varepsilon_0 \cdot [D_0 \varepsilon]_0 \cdot [D_0 \varepsilon_y]_0 \cdot \varepsilon_{yy,0} \\
& + 40320 \left( \sum_j \tau_{1j} (\rho_1 T_{10} T_{j1} + \rho_1 T_{11} T_{j0} + \rho_j T_{10} T_{j1}) \right) \varepsilon_0 \cdot [D_0 \varepsilon]_0 \cdot \varepsilon_{y,0} \cdot [D_0 \varepsilon_{yy}]_0 \\
& + 20160 T_{10} T_{11}^2 \varepsilon_0 [D_0 \varepsilon]_0^2 \cdot \varepsilon_{yyy,0} + 840 \rho_1^4 T_{10}^2 \varepsilon_0^2 [D_0^4 \varepsilon_{yy}]_0 \\
& + 10080 \left( \sum_j \tau_{1j} (\rho_1^2 T_{j0} + 2\rho_j^2 T_{10}) T_{j0} \right) \varepsilon_0^2 \cdot [D_0^2 \varepsilon_y]_0 \cdot \varepsilon_{yy,0} \\
& + 20160 \left( \sum_j \rho_1 \rho_j \tau_{1j} (2T_{10} + T_{j0}) T_{j0} \right) \varepsilon_0^2 [D_0 \varepsilon_y]_0 \cdot [D_0 \varepsilon_{yy}]_0 \\
& + 10080 \left( \sum_j \tau_{1j} (\rho_j^2 T_{j0} + 2\rho_1^2 T_{10}) T_{j0} \right) \varepsilon_0^2 \cdot \varepsilon_{y,0} [D_0^2 \varepsilon_{yy}]_0 \\
& + 20160 \left( \sum_{jk} \tau_{1j} (2\tau_{jk} T_{10} T_{k0} + 2\tau_{jk} T_{j0} T_{k0} + \tau_{1k} T_{j0} T_{k0} + \tau_{jk} T_{k0}^2) \right) \varepsilon_0^2 \cdot \varepsilon_{y,0}^2 \cdot \varepsilon_{yy,0} \\
& + 10080 T_{10}^2 T_{12} \varepsilon_0^2 \cdot [D_0^2 \varepsilon]_0 \cdot \varepsilon_{yyy,0} + 20160 \rho_1 T_{10}^2 T_{11} \varepsilon_0^2 \cdot [D_0 \varepsilon]_0 \cdot [D_0 \varepsilon_{yyy}]_0 \\
& + 3360 \rho_1^2 T_{10}^3 \varepsilon_0^3 [D_0^2 \varepsilon_{yy}]_0 + 20160 \left( \sum_j \tau_{1j} T_{10} T_{j0}^2 \right) \varepsilon_0^3 \cdot \varepsilon_{yy,0}^2 \\
& + 6720 \left( \sum_j \tau_{1j} (3T_{10}^2 + T_{j0}^2) T_{j0} \right) \varepsilon_0^3 \cdot \varepsilon_{y,0} \cdot \varepsilon_{yyy,0} \\
& + 1680 T_{10}^4 \varepsilon_0^4 \cdot \varepsilon_{yyyy,0}
\end{aligned}$$